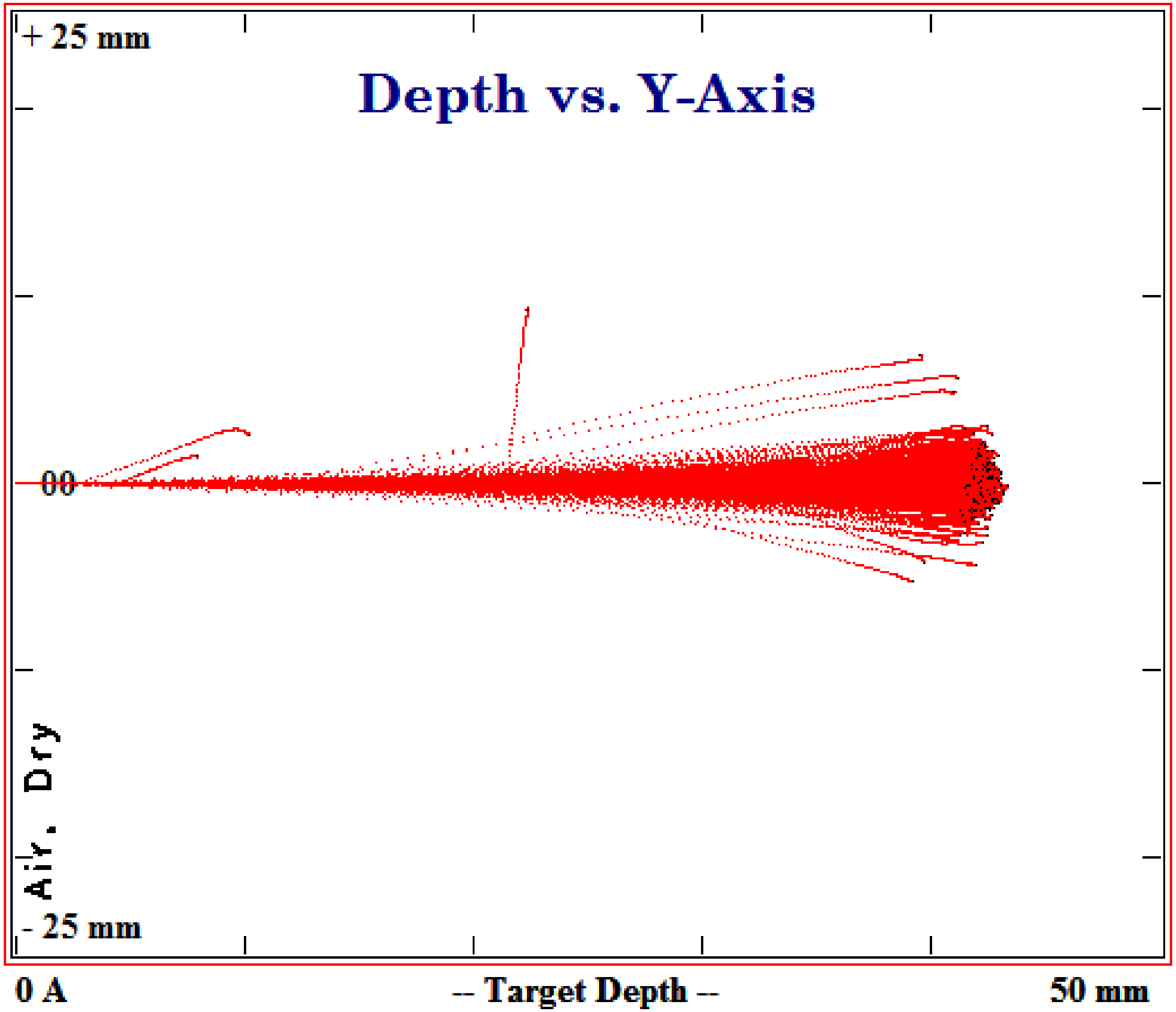
Chapter II:
Interactions of ions with matter

Trajectories of α particles of 5.5 MeV



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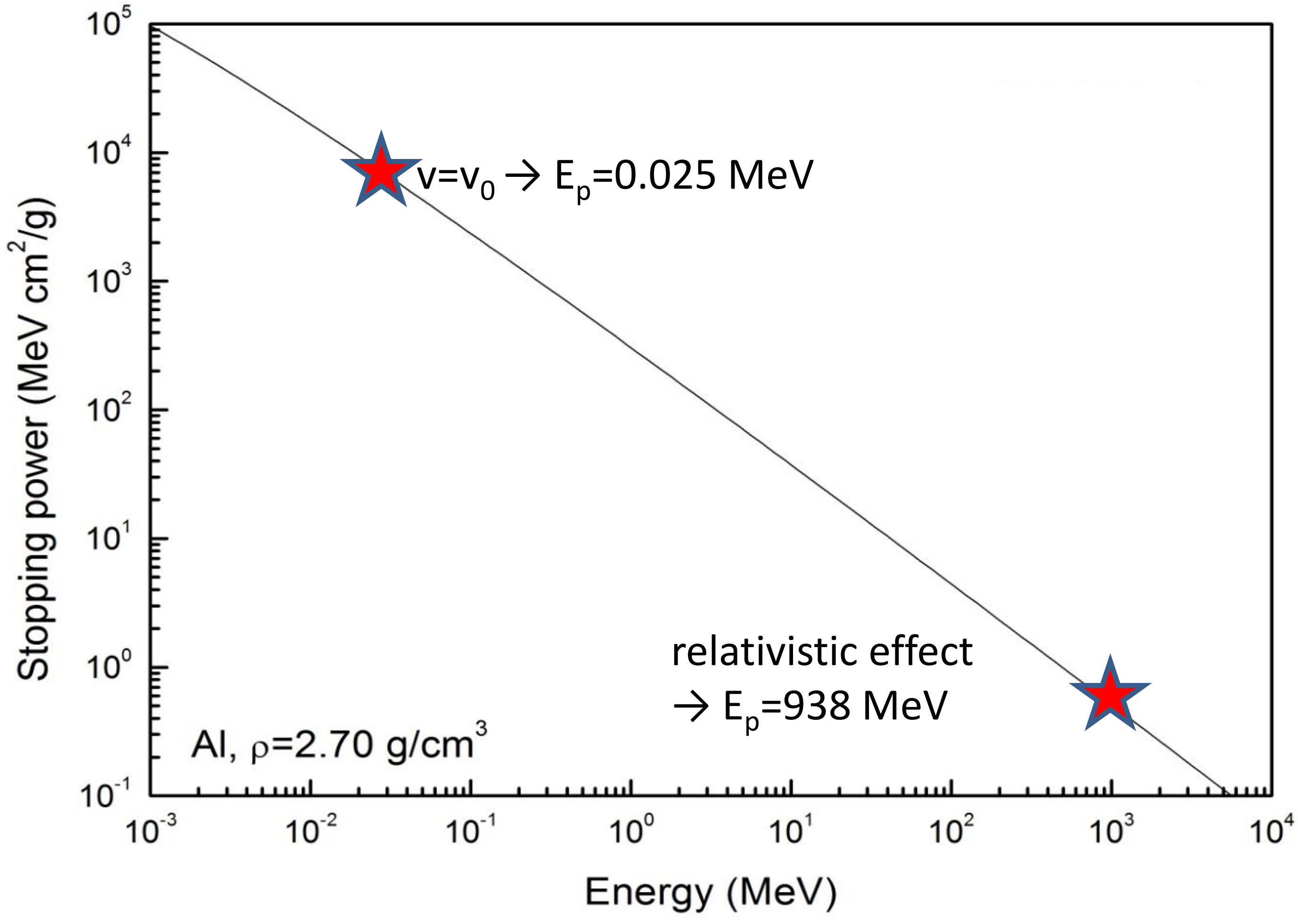
Incident proton on Al: Bohr model



Contents

- Quantum model of the electronic stopping force

  - Intermediate velocities

  - Large velocities

  - Small velocities

- Nuclear stopping force (small velocities)
- Range and Bragg curve

Transferred energy: Classical oscillator (1)

- Before to look for quantum processing → details about classical processing: electron = classical harmonic oscillator with pulsation ω_o → e^- bound to its site by a spring force with modulus $-m\omega_o^2 r$ → motion equation →

$$\frac{d^2\overrightarrow{r}}{dt^2} + \omega_0^2\overrightarrow{r} = -\frac{e}{m}\overrightarrow{E}(\overrightarrow{r}, t)$$

with $\overrightarrow{E}(\overrightarrow{r}, t)$ the electric field generated by the projectile (perturbation)

- No-linear equation → simplification →

$$\overrightarrow{E}(\overrightarrow{r}, t) = \overrightarrow{E}(\overrightarrow{r}(t), t) \equiv \overrightarrow{E}(t)$$

Transferred energy: Classical oscillator (2)

- By supposing the absence of electric field at $t = -\infty$ and $r(-\infty) = 0$ → a particular solution of the equation is →

$$\vec{r}(t) = -\frac{e}{m\omega_0}\int_{-\infty}^{t} dt' \vec{E}(t') \sin\omega_0(t-t')$$

- By supposing that the electric field ↘ after the distance of closest approach → it is possible to find a time t_1 for which the electric acting on the e^- becomes negligible → for $t > t_1$ → we can extend the maximal bound of the integration to $+\infty$ because the contributions of the integration are negligible for $t_1 < t' < +\infty$

Transferred energy: Classical oscillator (3)

- In this case the solution is →

$$\overrightarrow{r}(t) = -\frac{e}{m\omega_0}(\overrightarrow{C}\sin\omega_0 t - \overrightarrow{S}\cos\omega_0 t)$$

with

$$\overrightarrow{C} = \int_{-\infty}^{+\infty} dt'\,\overrightarrow{E}(t')\cos\omega_0 t' \quad \text{et} \quad \overrightarrow{S} = \int_{-\infty}^{+\infty} dt'\,\overrightarrow{E}(t')\sin\omega_0 t'$$

- To determine the energy lost by the projectile to the oscillator → determination of the electron velocity v_e →

$$\overrightarrow{v}_e(t) = -\frac{e}{m}(\overrightarrow{C}\cos\omega_0 t + \overrightarrow{S}\sin\omega_0 t)$$

Transferred energy: Classical oscillator (4)

- Thus the transferred energy *T* is →

$$T = -\frac{e^2}{2m}(\overrightarrow{C}^2 + \overrightarrow{S}^2)$$

- That can be also written →

$$T = -\frac{e^2}{2m}\left|\int_{-\infty}^{+\infty} dt'\,\overrightarrow{E}(t')e^{i\omega_0 t'}\right|^2$$

Classical oscillator: Dipolar approximation (1)

- We consider the Coulomb field generated by the incident particle →

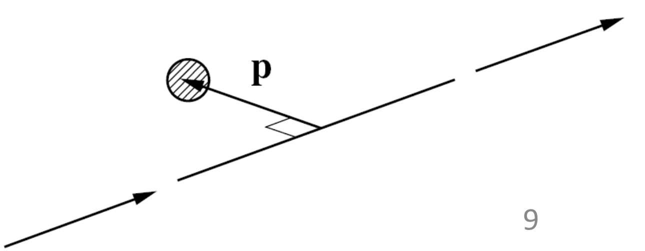
$$\overrightarrow{E}(\overrightarrow{r},t) = -\nabla\Phi(\overrightarrow{r},t)$$

with Φ, $\overrightarrow{R}$ and $\overrightarrow{v}$ the potential, trajectory and velocity of the particle:

$$\Phi(\overrightarrow{r},t) = \frac{e_1}{|\overrightarrow{r} - \overrightarrow{R}(t)|} \qquad \text{et} \qquad \overrightarrow{R} = \overrightarrow{p} + \overrightarrow{v}t$$

- We note that

$$\overrightarrow{p}.\overrightarrow{v} = 0$$



Classical oscillator: Dipolar approximation (2)

- We consider the Fourier transforms at 1 and 3 dimensions →

$$
\begin{aligned}
f(\omega) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} dt f(t) e^{-i\omega t} \\
f(\overrightarrow{q}) &= \frac{1}{(2\pi)^3}\int_{-\infty}^{+\infty} d^3\overrightarrow{r} f(\overrightarrow{r}) e^{-i\overrightarrow{q}.\overrightarrow{r}}
\end{aligned}
$$

- To obtain the Fourier transform of the potential → we use the relation →

$$\frac{1}{r} = \frac{1}{(2\pi)^2}\int_{-\infty}^{+\infty} d^3\overrightarrow{q}\,\frac{1}{q^2} e^{i\overrightarrow{q}.\overrightarrow{r}}$$

Classical oscillator: Dipolar approximation (3)

- The electric field can be thus written →

$$\vec{E}(\vec{r},t) = -\frac{ie_1}{(2\pi)^2}\int_{-\infty}^{+\infty} d^3\vec{q}\,\frac{\vec{q}}{q^2}e^{[i\,\vec{q}\,.(\vec{r}-\vec{p}-\vec{v}\,t)]}$$

- For small movements from the equilibrium → dipolar approximation →

$$e^{i\,\vec{q}\,.\,\vec{r}} \simeq 1 + i\,\vec{q}\,.\,\vec{r} \simeq 1$$

- The Fourier transform of the electric field can be written in the dipolar approximation →

$$\vec{E}(\omega) = -\frac{ie_1}{(2\pi)^2}\int_{-\infty}^{+\infty} d^3\vec{q}\,\frac{\vec{q}}{q^2}e^{-i\,\vec{q}\,.\,\vec{p}}\,\delta(\omega-\vec{q}\,.\,\vec{v})$$

Classical oscillator: Dipolar approximation (4)

- The integration is usually made by choosing the *x* axis along the projectile velocity and the *y* axis along the impact parameter →

$$\vec{E}(\omega) = -\frac{e_1\omega}{\pi v^2}\left(iK_0\left(\frac{\omega_{j0}p}{v}\right), K_1\left(\frac{\omega_{j0}p}{v}\right), 0\right)$$

with K_0 and K_1, the modified Bessel functions of order 0 and 1

- Thus *T* becomes →

$$T = \frac{2e_1^2e^2}{mv^2p^2} f_{dist}(p)$$

with

$$f_{dist}(p) = \left[\frac{\omega_0 p}{v} K_0\left(\frac{\omega_0 p}{v}\right)\right]^2 + \left[\frac{\omega_0 p}{v} K_1\left(\frac{\omega_0 p}{v}\right)\right]^2$$

- For $(\omega_0 p/v) \ll 1$ → $f_{dist} \simeq 1$ → we find again the Bohr result

Semi-classical model for the stopping power: $v_0 \ll v \ll c$ (1)

- Semi-classical model developed by Bethe (1930) → the motion of the nucleus is analyzed by classical mechanics and the motion of bound electrons by quantum mechanics → the electrons are no more considered as classical oscillators but occupy quantum states in the target atom
- We consider a target atom with Z_2 electrons (with mass m) and the stationary states $|j\rangle$ of energies ϵ_j, with j that represent a full set of quantum numbers and $j = 0$ for fundamental state → the resonant frequencies for an atom in its initial state are given by

$$\hbar\omega_{j0} = \epsilon_j - \epsilon_0$$

- The electrons are at rest during the → $v \gg v_0$

Semi-classical model for the stopping power: $v_0 \ll v \ll c$ (2)

- For a loss energy Q by the incident ion→ Bethe considered:

$$S = \sum_j \int Q d\sigma_R f_{j0}(Q)$$

- σ_R is the Coulomb cross section for a transferred energy Q (R is for Rutherford)
- The functions $f_{j0}(Q)$ are called generalized oscillator forces (GOS) that include all quantum effects for the stopping cross section and that describe the transition probabilities between different states for a given transferred energy Q
- Determination of $f_{j0}(Q)$?

Resolution of Schrödinger's equation (1)

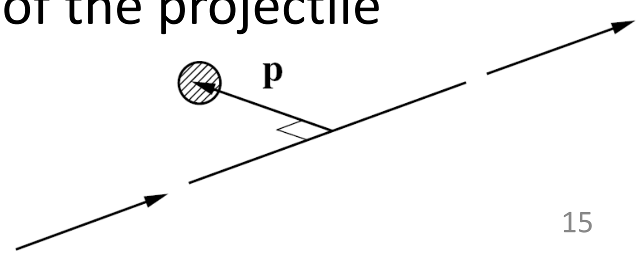
- The electronic motion is controlled by Schrödinger's equation depending on time →

$$(H+V)\Psi(\overrightarrow{r},t) = i\hbar\frac{d\Psi(\overrightarrow{r},t)}{dt}$$

with *H*, the Hamiltonian of an isolated atom of the target, Ψ, the wave function depending on time for a bound state of the atom, *V*, the potential describing the interaction with the given projectile is given by

$$V(\overrightarrow{r},t) = \sum_{\nu=1}^{Z_2}\frac{-e_1 e}{\overrightarrow{r}_\nu - \overrightarrow{R}(t)}$$

where $\overrightarrow{r}$ is for ($\overrightarrow{r}_1$,…. $\overrightarrow{r}_{Z_2}$) with $\overrightarrow{r}_\nu$ the position operator of the ν^{th} electron and $\overrightarrow{R} = \overrightarrow{p} + \overrightarrow{v}t$, the trajectory of the projectile



Resolution of Schrödinger's equation (2)

- The wave function depending on time Ψ can be developed according to stationary waves →

$$\Psi(\overrightarrow{r}, t) = \sum_j c_j(t) e^{-i\epsilon_j t} |j\rangle$$

where $|j\rangle$ are solutions of:

$$H|j\rangle = \epsilon_j |j\rangle$$

- Within the framework of the first order perturbations method (1st order Born approximation) → the c_j coefficients can be developed as power of the perturbation potential V →

$$c_j(t) = \delta_{j0} + c_j^{(1)}(t) + c_j^{(2)}(t) + ...$$

Resolution of Schrödinger's equation (3)

with

$$\delta_{j0} = \begin{cases} 1 & \text{for} \quad j = 0 \\ 0 & \text{for} \quad j \neq 0 \end{cases}$$

and

$$c_j^{(1)}(t) = \frac{1}{i\hbar} \int_{-\infty}^{t} dt' e^{i\omega_{j0} t'} \langle j | V(\overrightarrow{r}, t') | 0 \rangle$$

$$c_j^{(2)}(t) \quad = \quad \left(\frac{1}{i\hbar} \right)^2 \sum_k \int_{-\infty}^{t} dt' e^{i\omega_{jk} t'} \langle j | V(\overrightarrow{r}, t') | k \rangle$$

$$\times \int_{-\infty}^{t'} dt'' e^{i\omega_{k0} t''} \langle k | V(\overrightarrow{r}, t'') | 0 \rangle$$

and so on… (remark → fondamental state at t = - ∞)

Resolution of Schrödinger's equation (4)

- Within the framework of the first order perturbations method → only coefficients $c_j^{(1)}(\infty)$ are important → they are the transition amplitudes → important to calculate them
- By inserting in $c_j^{(1)}(\infty)$ the explicit expression of the potential, by considering the Fourier transform and by integrating on t' →

$$c_j^{(1)}(\infty) = \frac{-e_1 e}{i\pi\hbar} \int \overrightarrow{dq} \frac{e^{-i\overrightarrow{q}.\overrightarrow{p}}}{q^2} F_{j0}(\overrightarrow{q})\delta(\omega_{j0} - \overrightarrow{q}.\overrightarrow{v})$$

with

$$F_{j0}(\overrightarrow{q}) = \left\langle j \left| \sum_{\nu=1}^{Z_2} e^{i\overrightarrow{q}.\overrightarrow{r_\nu}} \right| 0 \right\rangle$$

We note $Q = \frac{\hbar^2 q^2}{2m}$

Transition probabilities

- The transition probabilities are given by (Postulate IV) →

$$P_j(p) = |\langle j|\Psi(\infty)\rangle|^2$$

- And thus within the framework of the first order perturbations method →

$$P_j(p) = \left|c_j^{(1)}(\infty)\right|^2$$

- Attention → $c_j^{(1)}(\infty) \neq 0$ for $\omega_{j0} < qv$ → condition son Q →

$$\omega_{j0}^2 < q^2 v^2 \Rightarrow 2mv^2 Q > (\epsilon_j - \epsilon_0)^2$$

Approximation of distant collisions – Dipolar approximation (1)

- We consider the $c_j^{(1)}(\infty)$ at large p (distant collisions) → we use the dipolar approximation →

$$e^{i\overrightarrow{q}.\overrightarrow{r}} \simeq 1 + i\overrightarrow{q}.\overrightarrow{r}$$

- We thus obtain

$$F_{j0}(\overrightarrow{q}) \simeq i\overrightarrow{q}\left\langle j\left|\sum_{\nu=1}^{Z_2}\overrightarrow{r_\nu}\right|0\right\rangle$$

- Within this approximation and choosing the x axis along the velocity of the projectile and the y axis along the impact parameter →

$$c_j^{(1)}(\infty) = -\frac{2e_1 e\omega_{j0}}{i\hbar v^2}\left\langle j\left|\sum_{\nu}^{Z_2}\overrightarrow{r}_\nu\right|0\right\rangle \times\left(iK_0\left(\frac{\omega_{j0}p}{v}\right), K_1\left(\frac{\omega_{j0}p}{v}\right), 0\right)$$

Approximation of distant collisions – Dipolar approximation (2)

with K_0 and K_1, the modified Bessel functions of 0 and 1 order

- The transitions probabilities thus become →

$$P_j(p) = -\frac{2e_1^2 e^2 Z_2}{mv^2 p^2 \hbar\omega_{j0}} f_{j0} \times \left\{ \left[\frac{\omega_{j0}p}{v} K_0\left(\frac{\omega_{j0}p}{v}\right)\right]^2 + \left[\frac{\omega_{j0}p}{v} K_1\left(\frac{\omega_{j0}p}{v}\right)\right]^2 \right\}$$

- The quantity f_{j0} is called the dipolar oscillator force and has as expression →

$$f_{j0} = \frac{2m}{3\hbar^2 Z_2}(\epsilon_j - \epsilon_0) \left| \left\langle j \left| \sum_{\nu}^{Z_2} \vec{r}_\nu \right| 0 \right\rangle \right|^2$$

with the sum rule of Thomas-Reiche-Kuhn: $\sum_j f_{j0} = 1$

Comparison classical ↔ semi-classical

- We consider the mean transferred energy T_{moy} as

$$T_{moy}(p) = \sum_j P_j(p)\hbar\omega_{j0}$$

- By comparing this expression with the classical result →

$$T = \frac{2e_1^2e^2}{mv^2p^2} f_{dist}(p)$$

$$f_{dist}(p) = \left[\frac{\omega_0 p}{v} K_0\left(\frac{\omega_0 p}{v}\right)\right]^2 + \left[\frac{\omega_0 p}{v} K_1\left(\frac{\omega_0 p}{v}\right)\right]^2$$

- Equal expression with

$$f_{dist}(p) = \sum_j f_{j0} \left[\frac{\omega_{j0} p}{v} K_0\left(\frac{\omega_{j0} p}{v}\right)\right]^2 + \left[\frac{\omega_{j0} p}{v} K_1\left(\frac{\omega_{j0} p}{v}\right)\right]^2$$

Beyond distant collisions

- To generalize the previous f_{j0} functions to large values of *Q*, Bethe sets out →

$$f_{j0}(Q) = \frac{1}{Z_2} \frac{\epsilon_j - \epsilon_0}{Q} |F_{j0}(\vec{q})|^2$$

called generalized oscillator forces

- At the limit of small *Q* values →

$$f_{j0}(Q)\Big|_{Q \simeq 0} = f_{j0}$$

Stopping power: Bethe equation: $v_0 \ll v \ll c$ (1)

- Necessary distinction between distant and close collisions (via *p*) $\leftrightarrow$ collisions with large or small transferred momentum (via *q*) $\leftrightarrow$ collisions with or small transferred energy (via *Q*)
- Splitting of the integral:

$$S = \sum_j \int Q d\sigma_R f_{j0}(Q)$$

into 2 parts in relation to Q_0 → For $Q < Q_0$ → dipolar approximation is valid (Q_0) →

$$S_{dist} = \sum_j f_{j0} \int_{(\epsilon_j - \epsilon_0)^2/2mv^2}^{Q_0} Q d\sigma_R$$

Stopping power: Bethe equation: $v_0 \ll v \ll c$ (2)

- For $Q > Q_0$ → it is necessary to determine the upper bound of the integral → for an ion interacting with an e⁻ ($m_1 \gg m$) →

$$\begin{aligned} T_{max} &= \gamma E \\ &= \frac{4 m_1 m}{(m_1 + m)^2} \frac{m_1 v^2}{2} \\ &\simeq 2 m v^2 \end{aligned}$$

- That gives →

$$S_{close} = \int_{Q_0}^{2mv^2} Q d\sigma_R \sum_j f_{j0}(Q)$$

Stopping power: Bethe equation: $v_0 \ll v \ll c$ (3)

- Bethe demonstrated that →

$$\sum_j f_{j0}(Q) = 1$$

- We have thus →

$$S_{close} = \int_{Q_0}^{2mv^2} Q d\sigma_R \equiv \sum_j f_{j0} \int_{Q_0}^{2mv^2} Q d\sigma_R$$

- By combining close and distant collisions →

$$S = S_{close} + S_{dist} = \sum_j f_{j0} \int_{(\epsilon_j - \epsilon_0)/2mv^2}^{2mv^2} Q d\sigma_R$$

Stopping power: Bethe equation : $v_0 \ll v \ll c$ (4)

- By considering the explicit expression of $d\sigma_R \rightarrow$

$$d\sigma_R = 2\pi \frac{e_1^2 e_2^2}{m_2 v^2} \frac{dQ}{Q^2}$$

- We thus obtain

$$S = \frac{4\pi e_1^2 e^2}{m v^2} Z_2 \sum_j f_{j0} \ln \frac{2 m v^2}{\epsilon_j - \epsilon_0}$$

Stopping power: Bethe equation: $v_0 \ll v \ll c$ (5)

- The stopping power equation of Bethe is usually written →

$$\boxed{S_e = \frac{4\pi e_1^2 e^2}{mv^2} Z_2 \ln \frac{2mv^2}{I}}$$

with *I* defined as the mean excitation energy such as →

$$\ln I = \sum_j f_{j0} \ln \left(\epsilon_j - \epsilon_0\right)$$

- Let's recall the application conditions →

$$\begin{aligned} m_1 &\gg m \\ v &\gg v_0 \Rightarrow mv^2 \gg \hbar\omega_0 \end{aligned}$$

Bethe equation versus Bohr equation

$$S_e = \frac{4\pi Z_2 e_1^2 e^2}{mv^2} L_e$$

$$\text{with} \qquad L_e = \ln \frac{Cmv^3}{|e_1 e|\omega_0} \quad \text{from Bohr}$$

$$\text{with} \qquad L_e = \ln \frac{2mv^2}{I} \quad \text{from Bethe}$$

Principal dependences of the stopping force

$$-\left(\frac{dE}{dx}\right)_{elec} = NS_e = \frac{4\pi e_1^2 e^2}{mv^2} NZ_2 \ln\frac{2mv^2}{I}$$

$\frac{4\pi e_1^2 e^2}{mv^2}$ Principal dependence in the velocity

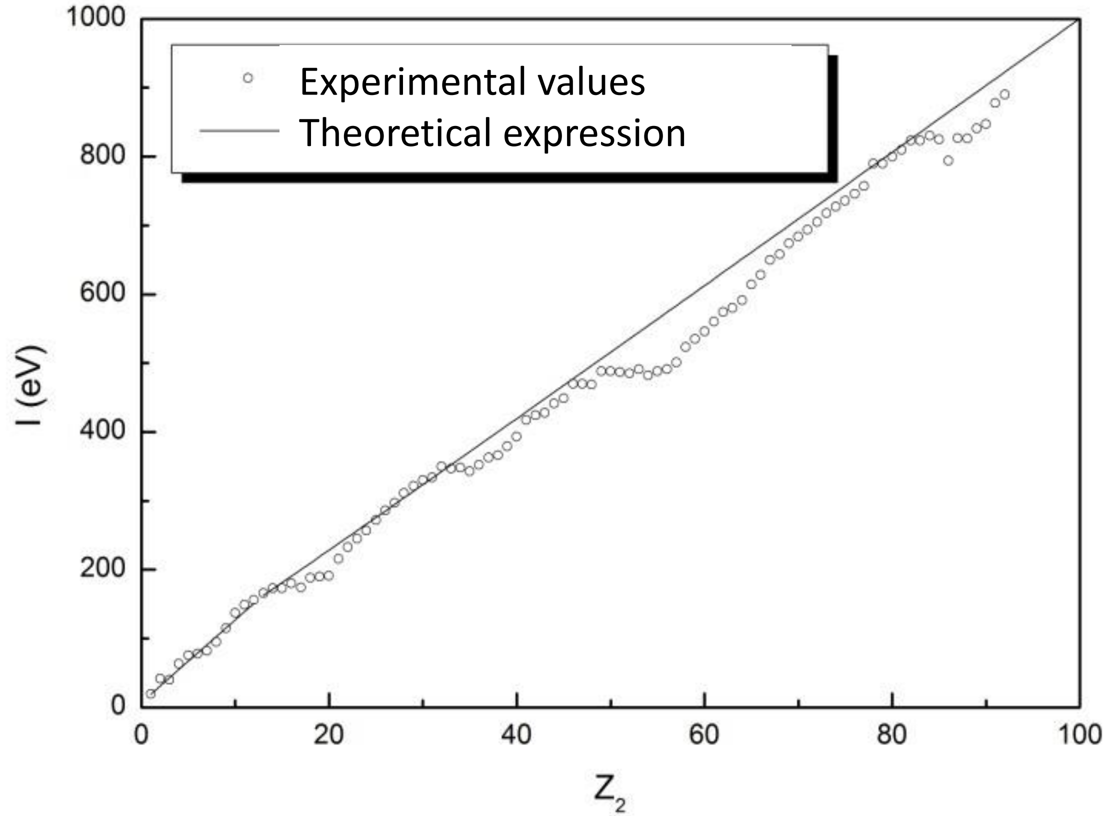
NZ_2 Principal dependence in the material

$\ln\frac{2mv^2}{I}$ Weak dependence in the velocity and in the material

Mean logarithmic excitation energy (1)

- The mean logarithmic excitation energy *I* only depends on the medium (not on the projectile)
- Difficult calculations → obtained from experiment
- *I* is in the logarithmic part of → not necessary to be known with precision
- *I* linearly varies (approximately) with *Z* → atomic model of Thomas-Fermi (atomic electrons = "gas")
- The irregularities in the variation with *Z* are due to the shell structure of the atom
- Usually → evaluation of *I* with an empirical equation

Mean logarithmic excitation energy (2)



$$\frac{I}{Z} = \begin{cases} 12 + 7/Z & Z < 13 \\ 9.76 + 58.8 Z^{-1.19} & Z \geq 13 \end{cases}$$

I for composite materials

- For composite materials → the stopping power of the material can be approximated by the sum of the stopping powers of its elementary constituents → identical relation for the mean excitation energies
- Bragg's additivity rule for *n* materials *i*:

$$NZ = \sum_i^n N_i Z_i$$

$$NZ \ln I = \sum_i^n N_i Z_i \ln I_i$$

- Z_i is the atomic number of the atoms of type *i*, N_i is the number of atoms of type *i* per volume unit and $N = \sum_i N_i$ is the total number of atoms per volume unit

Approximate rule → can lead to important mistakes

Bethe-Bloch equation: $v_0 < v \simeq c$ (1)

Many corrections to the Bethe equations → Bethe-Bloch equations (in the Born approximation)

$$\boxed{S_e = \frac{4\pi r_e^2 mc^2}{\beta^2} Z z^2 L(\beta)}$$

Standard reference expression for the electronic stopping power with $\beta = v/c$, $z = e_1/e$, $r_e = e^2/(mc^2)$ (r_e: classical radius of the electron)

$$\boxed{L(\beta) = L_0(\beta) = \frac{1}{2}\ln\left(\frac{2mc^2\beta^2 W_m}{1-\beta^2}\right) - \beta^2 - \ln I - \frac{C}{Z} - \frac{\delta}{2}}$$

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Bethe-Bloch equation: $v_0 < v \simeq c$ (2)

- With W_m the maximum energy transferred during 1 collision to a free electron (non-approximated relativistic expression) →

$$W_m = \frac{2mc^2\beta^2}{1-\beta^2}\left[1 + \frac{2m}{m_1(1-\beta^2)^{1/2}} + \left(\frac{m}{m_1}\right)^2\right]^{-1}$$

- For $m_1 \gg m$ → we well find $2m\gamma_1^2 v^2$

Relativistic correction: $v \simeq c$ (1)

- When $v \simeq c$ or $\beta = v/c \simeq 1$→ relativistic corrections have to be done to previous expression → term $\gamma_1 = (1-\beta^2)^{-1/2}$
- We also have → $p_{max} \sim \gamma_1 v/\omega_0$ → ↗ of the upper bound of the impact parameter when v ↗
- A complete relativistic classical calculation (as for quantum) shows that *E* becomes →

$$\vec{E}(\omega) = -\frac{e_1\omega}{\pi\gamma_1 v^2}\left(\frac{i}{\gamma_1}K_0\left(\frac{\omega_{j0}p}{\gamma_1 v}\right), K_1\left(\frac{\omega_{j0}p}{\gamma_1 v}\right), 0\right)$$

- We have thus a relativistic modification of $f_{dist}(p)$ →

$$f_{dist}(p) = \frac{1}{\gamma_1^2}\left[\frac{\omega_0 p}{\gamma_1 v}K_0\left(\frac{\omega_0 p}{\gamma_1 v}\right)\right]^2 + \left[\frac{\omega_0 p}{\gamma_1 v}K_1\left(\frac{\omega_0 p}{\gamma_1 v}\right)\right]^2$$

Relativistic correction: $v \simeq c$ (2)

- And thus a modification of the principal dependence in velocity →

$$\frac{4\pi e_1^2 e^2}{mv^2} \Rightarrow \frac{4\pi e_1^2 e^2}{m\gamma_1^2 v^2} = \frac{4\pi e_1^2 e^2}{mv^2}(1-\beta^2)$$

- Moreover the momentum of the incident particle becomes $m\gamma_1 v$ →

$$T_{max} = 2m\gamma_1^2 v^2$$

- And thus we have a modification of the logarithmic term →

$$\ln\frac{2mv^2}{I} \Rightarrow \ln\frac{2m\gamma_1^2 v^2}{I} = \ln\frac{2mv^2}{I(1-\beta^2)}$$

- The combination of all modifications implies that <u>S ↗ when v ↗</u>

Density correction (1)

- Density correction → -δ/2
- In the Bethe equation → interactions with isolated atoms → valid for low density gas
- In condensed matter (solid) → the interactions can get done with a large amount of atoms at once → we have to consider collective effects
- Model of Fermi (1940) → matter assimilated to a gas of oscillators submitted to the electric field of the particle
- Incident charged particle → polarization of matter → the electric field due to the charged particle disturb the atoms → they get a dipolar electric momentum → production of an electric field opposed to the field due to the charged particle → reduction of the electric field due to screening effect of the dipoles

Density correction (2)

- The polarization implies that distant atoms are submitted to a weaker electric field → their contribution to the stopping power is then reduced
- The density effect particularly appears for high energies because of the factor γ_1 in p_{max} that increases the mistake made by ignoring polarization of the medium → v ↗ → p_{max} ↗ → $\delta/2$ ↗ → S ↘
- The density correction can be written →

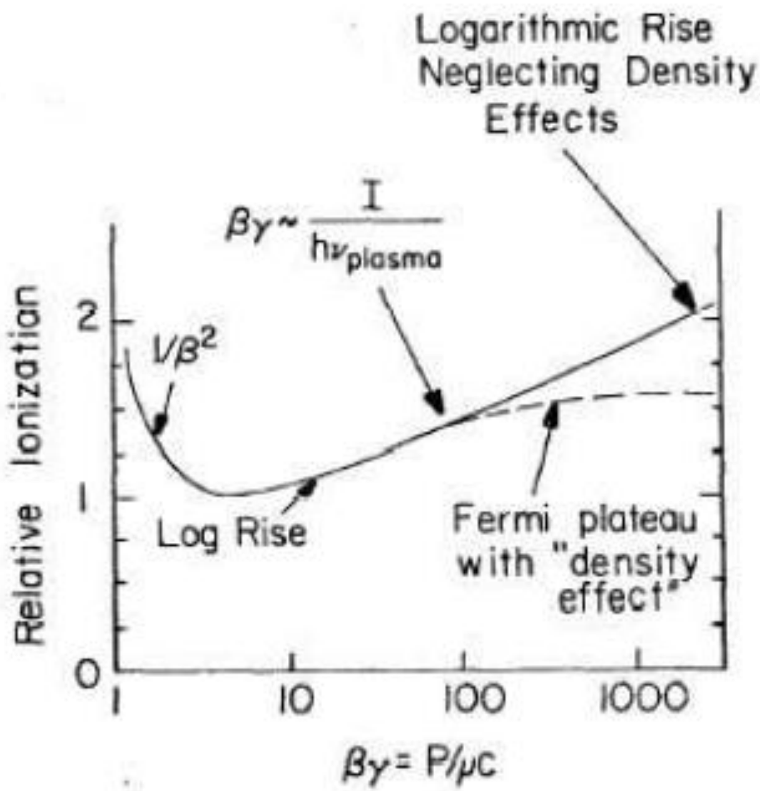
$$\frac{\delta}{2} = \ln \frac{\hbar \omega_p}{I} + \ln \gamma_1 \beta - \frac{1}{2}$$

with ω_p, the plasma pulsation for an electronic density $n = NZ$ (ϵ_0: dielectric constant) →

$$\omega_p = \sqrt{\frac{ne^2}{\epsilon_0 m}}$$

Density correction (3)

- Relativistic and density corrections cancel each other out→ Fermi's plateau



Shell correction (1)

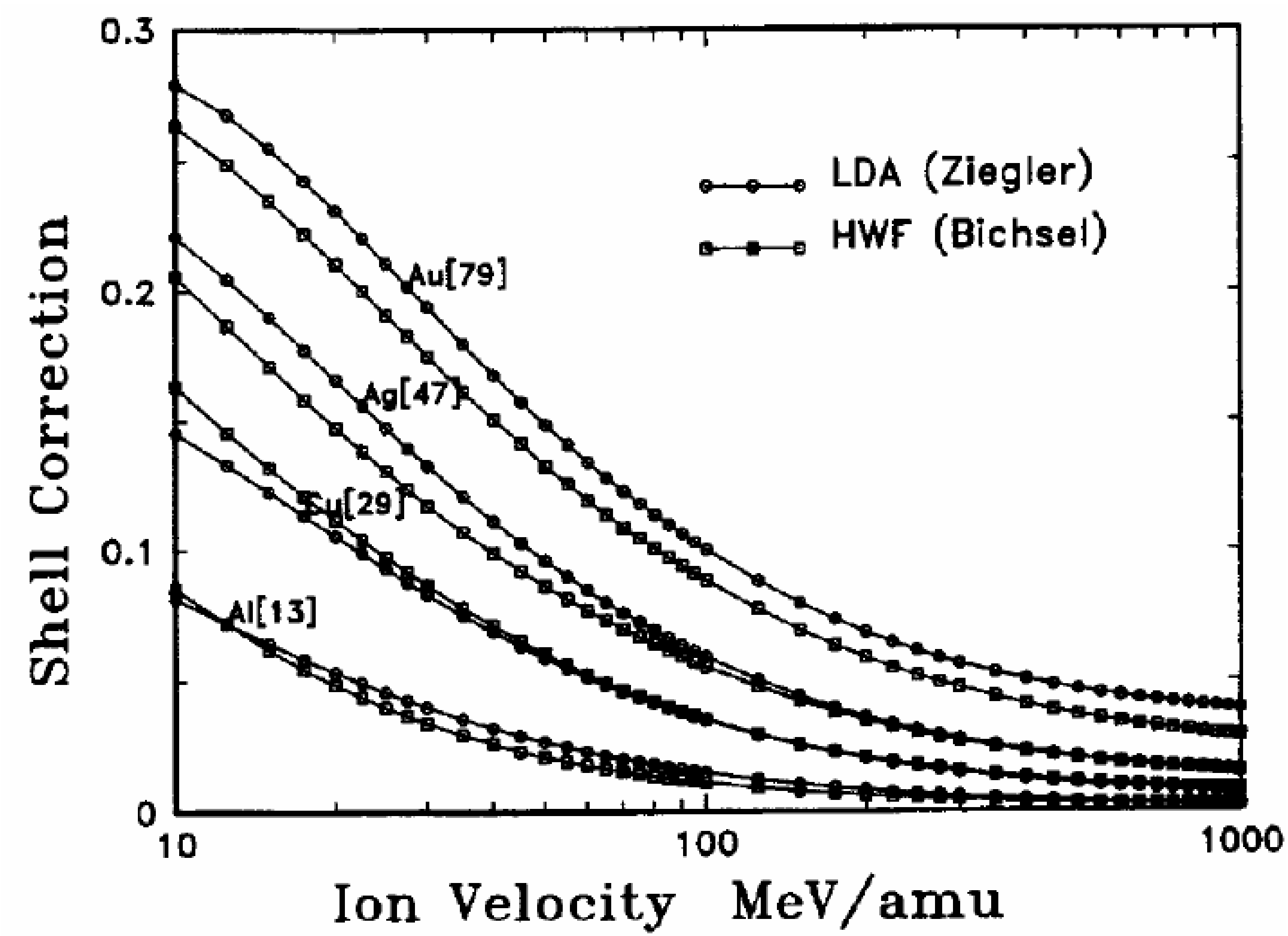
- Shell correction → -C/Z
- Bethe and Bohr equations supposed v $\gg$ v_0 (velocity of the atomic electrons) → the evaluation of *I* is based on this assumption → mean *I* value
- When it is not the case (v ↘) → it is necessary to explicitly calculate the ions-electrons interactions for each electron shell and for each electron binding energy
- When v ↘ → contribution to *S* of internal electrons (first K, then L, …) ↘
- "Mean" correction that reduces S (maximal correction = 6%) → = for all charged particles (including electrons) → only dependent on medium and velocity

Shell correction (2)

- 2 models to calculate *C/Z* →

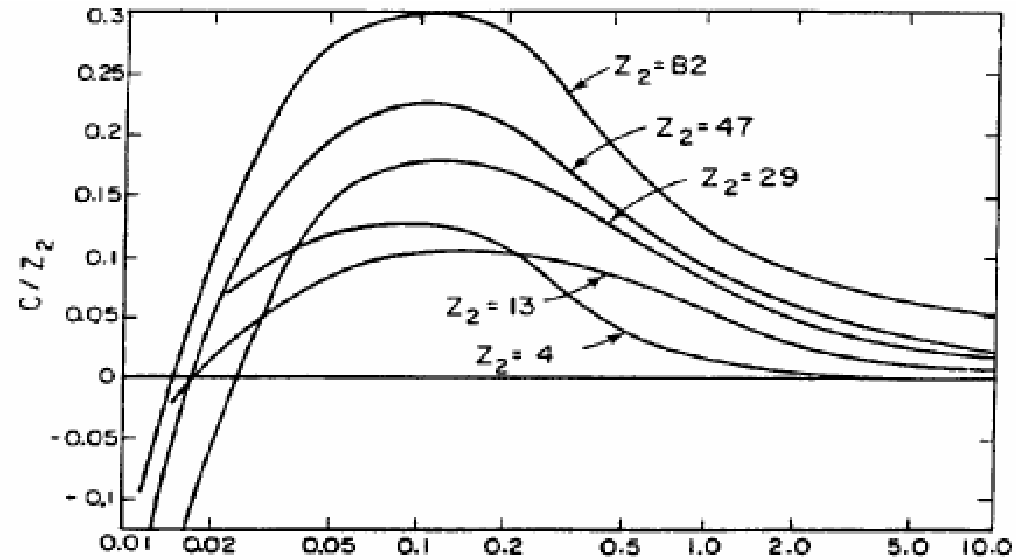
1. The method of the hydrogenous wave functions (HWF: bound e^- described by hydrogenous wave functions)
2. The method of the local density approximation (LDA: bound e^- are a gas of e^- with variable density)

Shell correction (3)

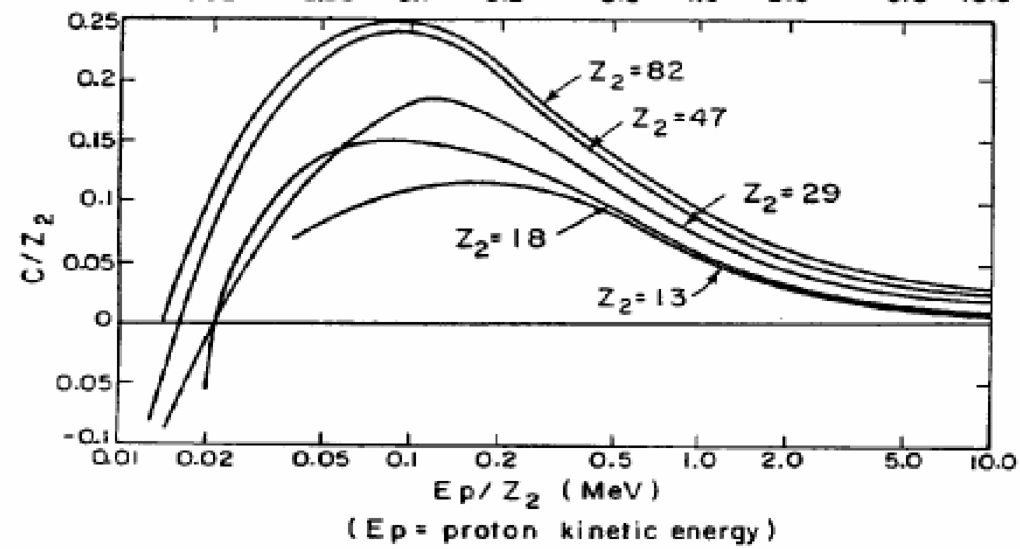


Shell correction (4)

LDA



HWF



Corrections beyond the first order Born approximation

- The stopping number L_0 is valid only if the velocity of the projectile is large by comparison to the velocities of the atomic electrons
- For $v_0 \lesssim v$ → the first order Born approximation (necessary for the calculations of Bethe) is no more valid
- We have to add correction terms to L_0 → expansion of L in power of z →

$$\boxed{L(\beta) = L_0(\beta) + zL_1(\beta) + z^2 L_2(\beta)}$$

Barkas-Andersen correction

- Barkas-Andersen correction → $zL_1(\beta)$

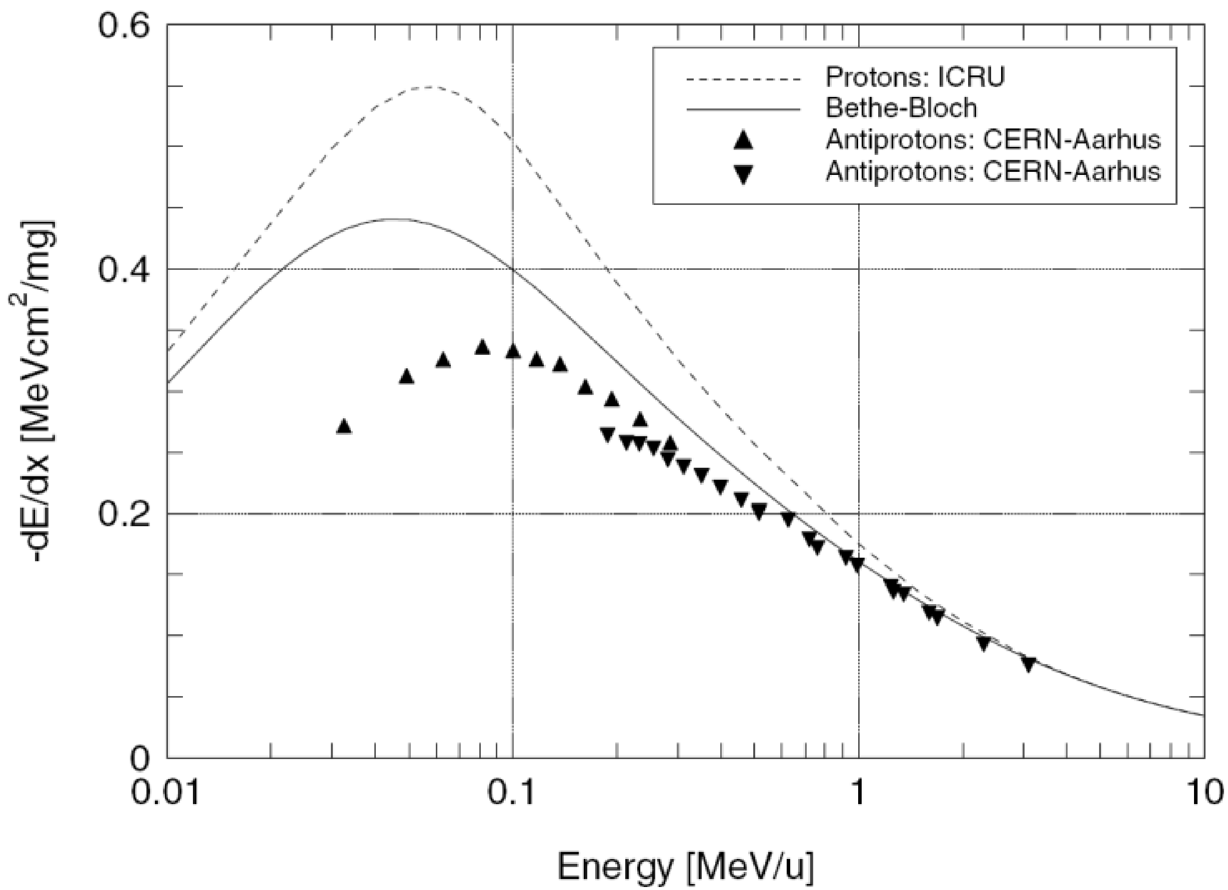
- The Barkas-Andersen correction is proportional to an odd power in z (charge of the projectile) → *S* for negative particles is slightly weaker than for positive particles → S≠ between particles and corresponding antiparticles

- A positive charge attracts the e^- → the interactions ↗ → S ↗

- A negative charge repulses the e^- → the interactions ↘ → S ↘

Example of Barkas-Andersen effect

Incident proton and antiprotons on silicon



Bloch correction

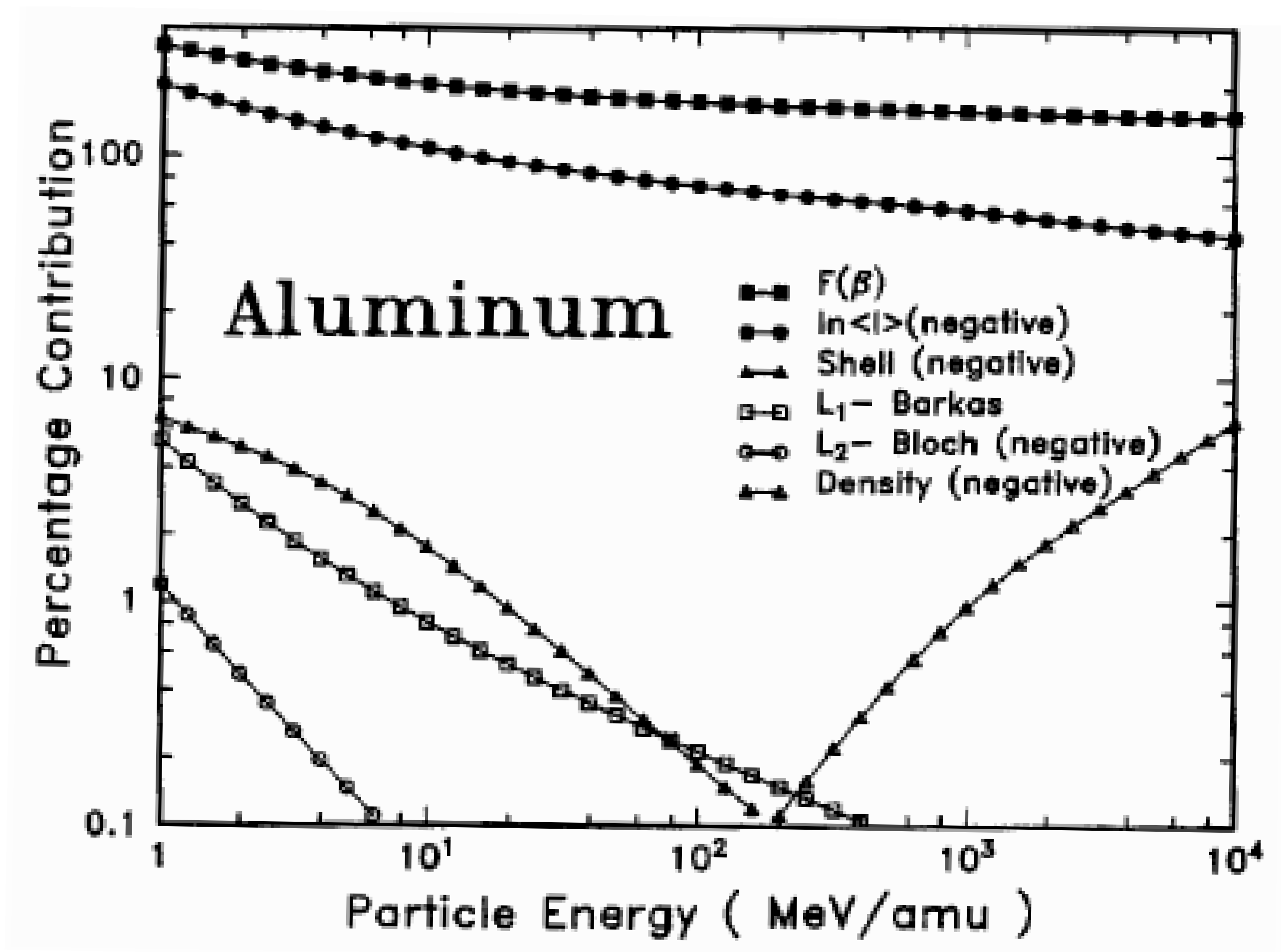
- Bloch correction → $z^2L_2(\beta)$
- Semi-classical model taking precisely into account distant collisions (large impact parameter)
- Generally Bichsel evaluation of the Bloch correction is used:

$$z^2 L_2(y) = -y^2[1.202 - y^2(1.042 - 0.855y^2 + 0.343y^4)]$$

where $y=z\alpha/\beta$ and α=1/137 (fine structure constant)

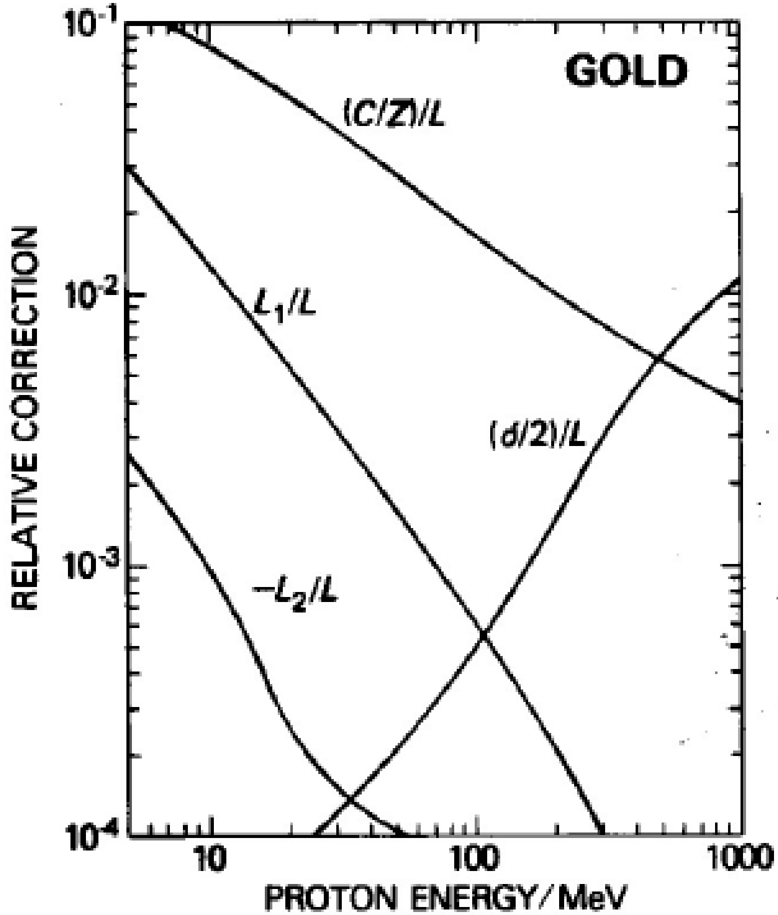
Evaluation of various corrections (1)

Incident proton on aluminium



Evaluation of various corrections (2)

Protons incident on gold →



Stopping cross section for ions at very high velocities

Ultra-relativistic equation of Lindhard-Sørensen (E$\sim$ 100 GeV: far beyond normal applications)

$$\boxed{L \rightarrow \ln \frac{1.64c}{R\omega_p}}$$

R: radius of the projectile, ω_p=$(4\pi\ e^2 N_e/m)^{1/2}$: plasma frequency that quantifies the electronic density

Attention: for E $\nearrow$ the creation of electron-positron pairs becomes predominant

Electronic cross section for ions at small velocities

$v \lesssim v_0$ → Perturbation theory not applicable (no sudden collision)

Moreover electrons capture by incident projectiles (for example: He^{++} → He^{+} → He^{0}) → charge state of the ion is variable (Thomas-Fermi theory):

$$z^* = z\left(1 - e^{-v/(z^{2/3}v_0)}\right)$$

Different theories but not so precise that the Bethe-Bloch theory for large velocities → use of semi-empirical expressions based on a theoretical « trend »

$$\Rightarrow \boxed{S_e \propto E^{0.5}}$$

Nuclear cross section for ions at small velocities (1)

- Chapter 1 → Nuclear collisions for incidents ions are rare → small contribution to the total stopping power

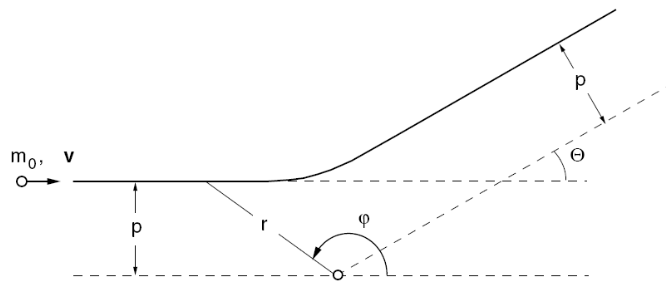
- Only for incident ions with small velocity → even in that case their contribution is small

- However → They can have effects a posteriori → radiative damages

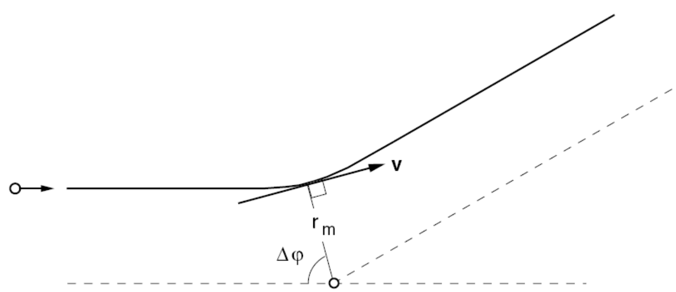
Nuclear cross section for ions at small velocities (2)

in the center of mass system:

diffusion by angle θ due to a un central potential V(r)



(a) Definition of variables



(b) Distance of closest approach

$$\Rightarrow \quad S_n = \int T d\sigma = \int T 2\pi p dp = 2\pi\gamma E \int \sin^2(\theta/2) p dp \quad \text{with} \quad \gamma = \frac{4m_1 m_2}{(m_1+m_2)^2}$$

Nuclear cross section for ions at small velocities (3)

$$\frac{m_0}{2}\left[\left(\frac{dr}{dt}\right)^2 + r^2\left(\frac{d\varphi}{dt}\right)^2\right] + V(r) = \frac{m_0}{2}v^2 \equiv E_r$$

$$m_0 r^2 \frac{d\varphi}{dt} = -m_0 p v$$

$$\Rightarrow \theta = \pi - 2\int_{r_m}^{\infty} dr\, \frac{p}{r^2}\left(1 - \frac{V(r)}{E_r} - \frac{p^2}{r^2}\right)^{-1/2}$$

with E_r the initial kinetic energy of the relative motion

Nuclear cross section for ions at small velocities (4)

Interaction potential: $V(r) = \frac{z_1 Z_2 e^2}{r} F_s(\frac{r}{r_s})$

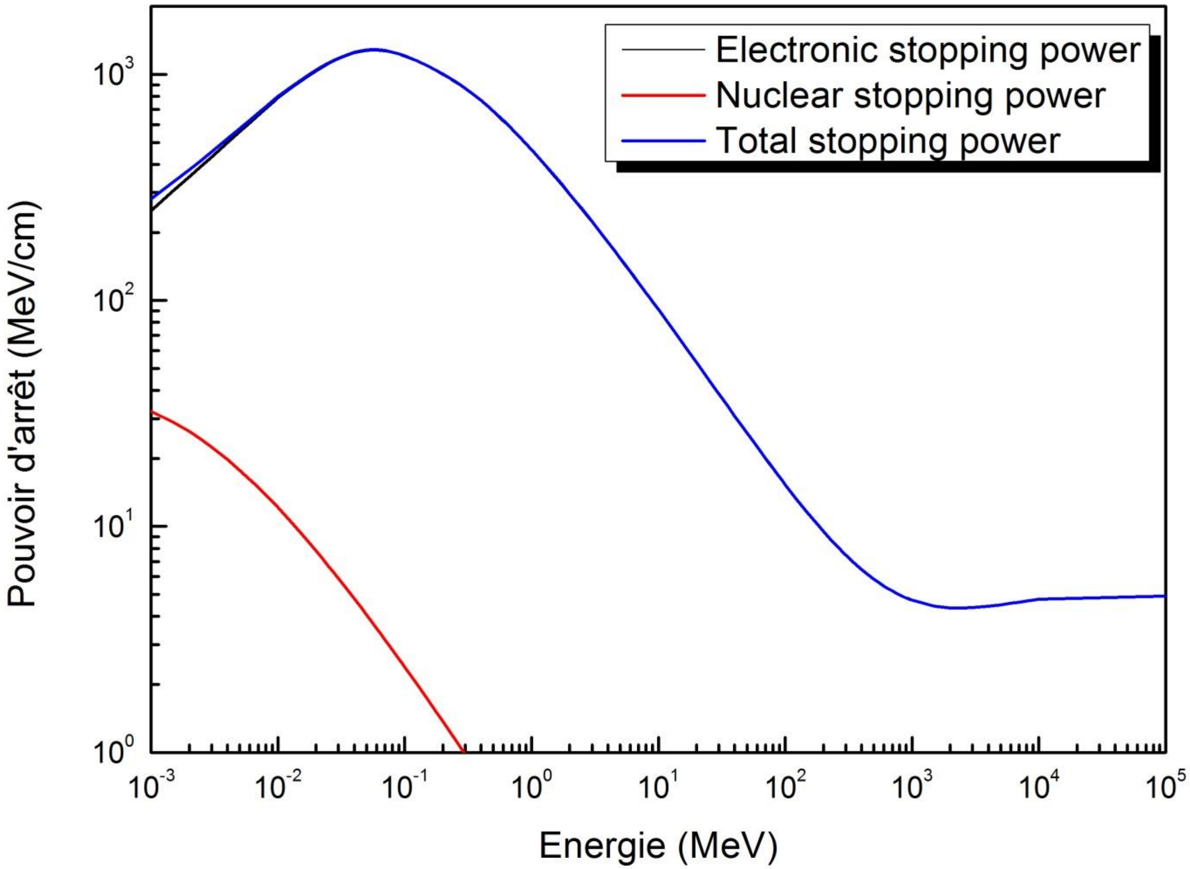
The screening function $F_s(r/r_s)$ takes into account the screening by the atomic electrons (r_s: screening length in the model of Thomas-Fermi) → Adjustment to experimental results → « universal screening function »

$$\begin{aligned} F_s(r/r_s) \quad = \quad & 0.1818 \exp\left(-3.2 r/r_s\right) + 0.5099 \exp\left(-0.942 r/r_s\right) \\ & + 0.2802 \exp\left(-0.4029 r/r_s\right) + 0.2817 \exp\left(-0.2016 r/r_s\right) \end{aligned}$$

with $r_s = 0.88534 a_0 \left(z_1^{0.23} + Z_2^{0.23}\right)^{-1}$ and $a_0 = 0.529 \text{Å}$

Stopping power for ion: example

Incident proton on aluminium → $S = S_{elec} + S_{nucl} \approx S_{elec} = S_{coll}$



Electronic mass stopping power (1)

- Mass stopping power: ratio between the stopping power and the density ρ of the material (ordinary unit: MeV cm^2 g^{-1}) →

$$\frac{NS(E)}{\rho} = -\frac{1}{\rho}\frac{dE}{dx}$$

- With $\rho = M_A N/N_A$ (M_A is the molar mass, N is the atomic density and N_A is the Avogadro number) and $M_A = AM_u$ (A is le mass number and $M_u = m_u N_A = 10^{-3}$ kg mol^{-1} is the constant of molar mass and m_u is the atomic mass constant) →

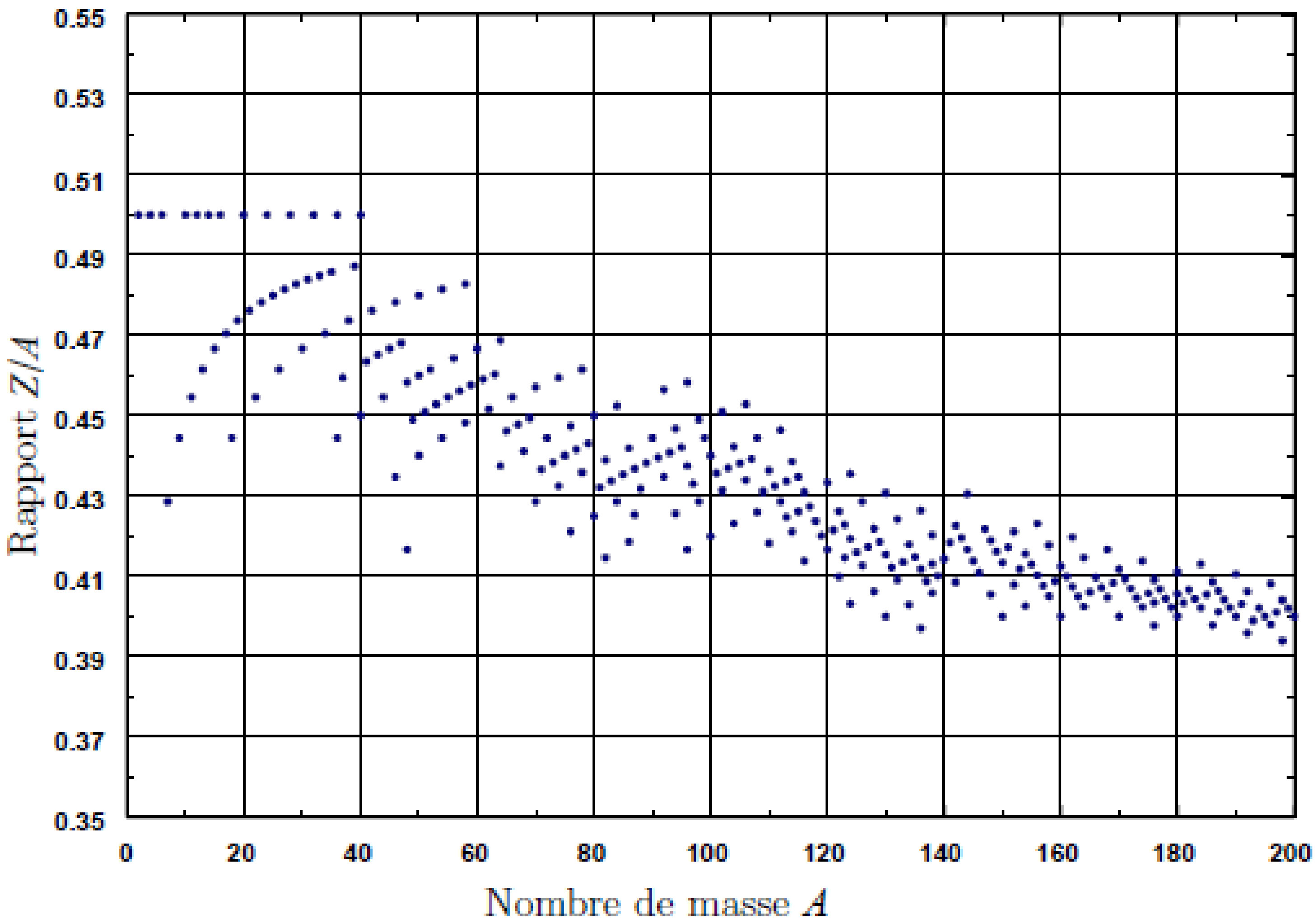
$$\boxed{-\frac{1}{\rho}\frac{dE_{elec}}{dx} = 4\pi r_e^2 mc^2 \frac{N_A}{M_u}\frac{Z}{A}\frac{z^2}{\beta^2}L(\beta)}$$

Electronic mass stopping power (2)

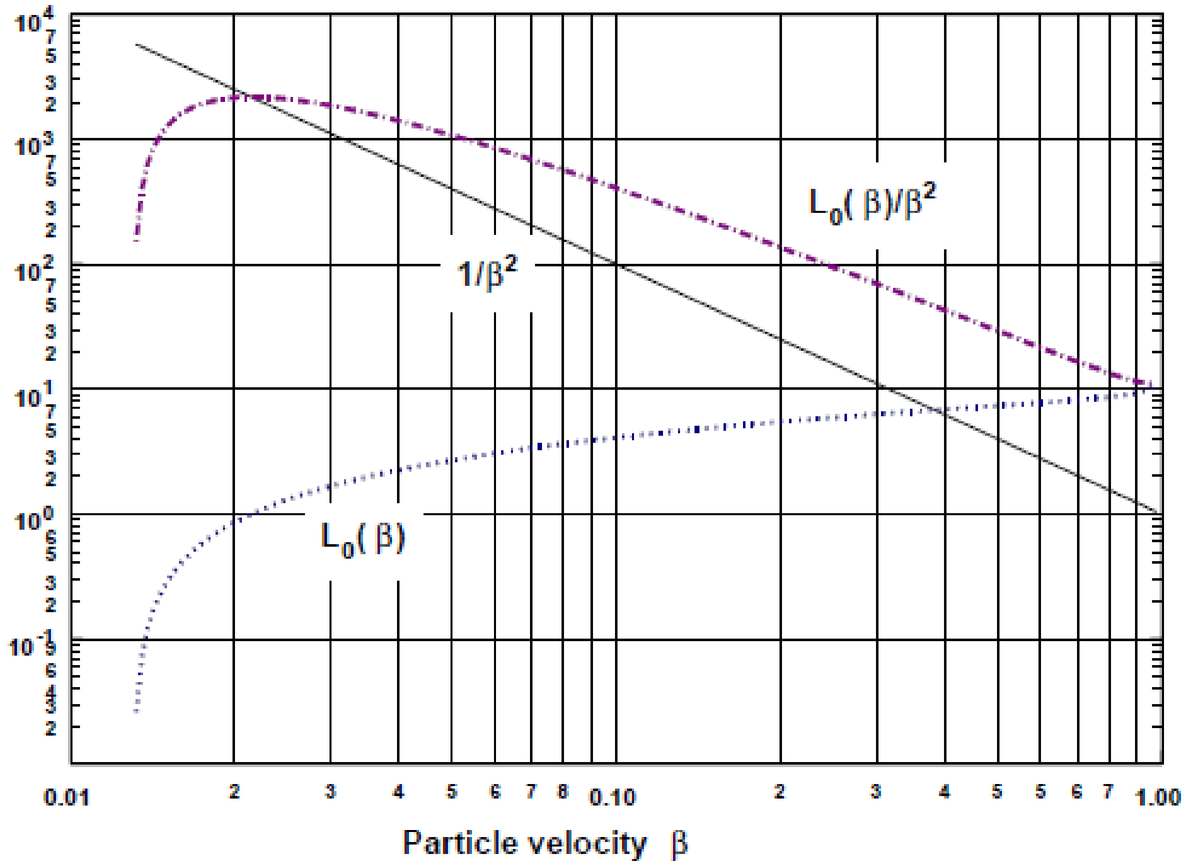
The electronic mass stopping power is the product of 4 factors:

1. The constant factor $4\pi r_e^2 mc^2 N_A/M_u$ = 0.307 MeV cm^2 g^{-1} → order of magnitude for the electronic mass stopping power
2. The factor *Z/A* that is included between 0.4 et 0.5 for all stable isotopes (except hydrogen) → weak dependency into the medium
3. The factor β^{-2} → monotonic decreasing function in ion velocity that tends to 1 for large energies → explain the decrease of the stopping power as a function of the energy
4. The stopping number $L(\beta)$ → for $L(\beta) = L_0(\beta)$ → monotonic increasing function (slow) in the velocity and in *Z* (via *I*: $-\ln I$)

Variation of Z/A as a function of A

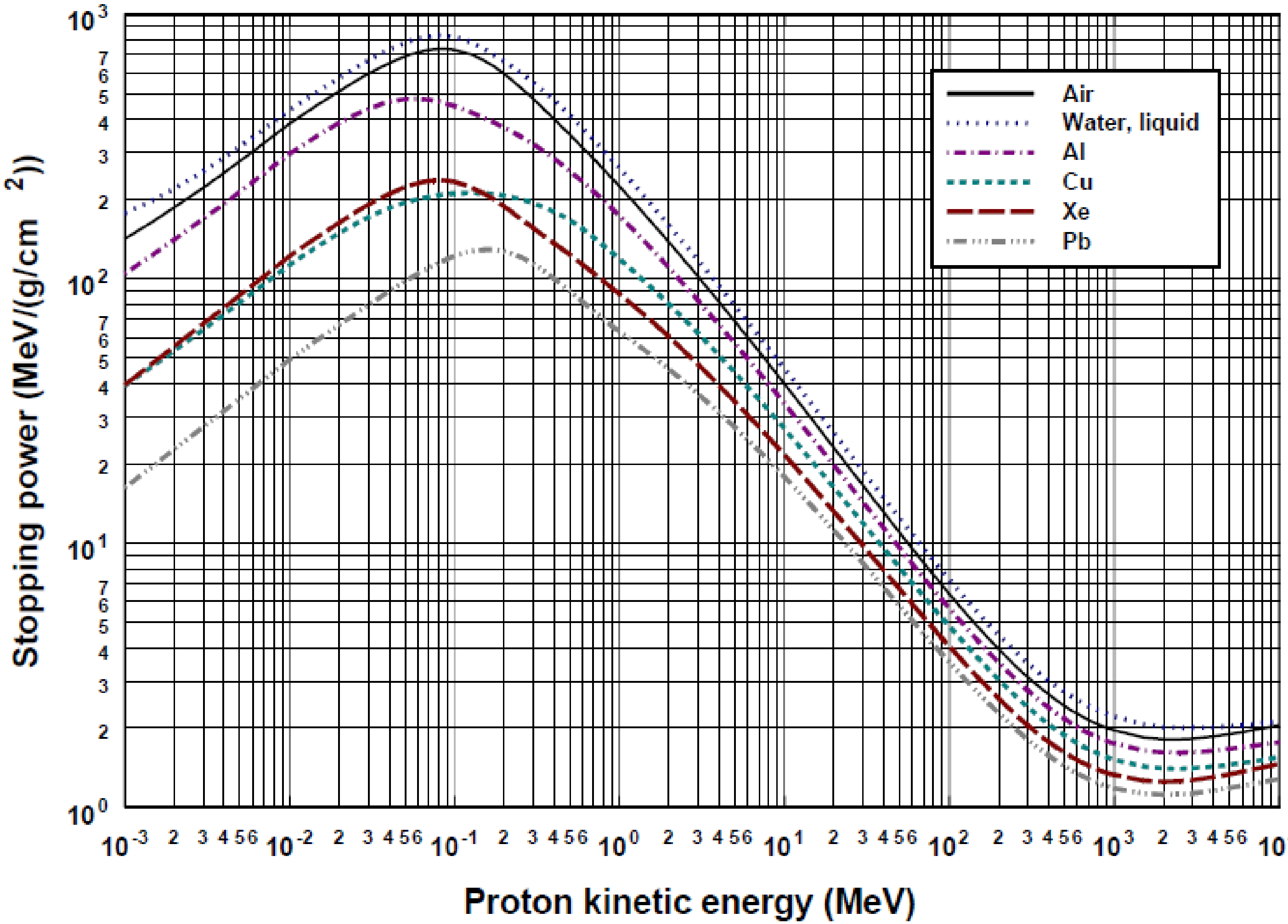


Velocity dependency



Protons incident on Si → shell and density corrections are neglected in the calculation of $L_0(\beta)$

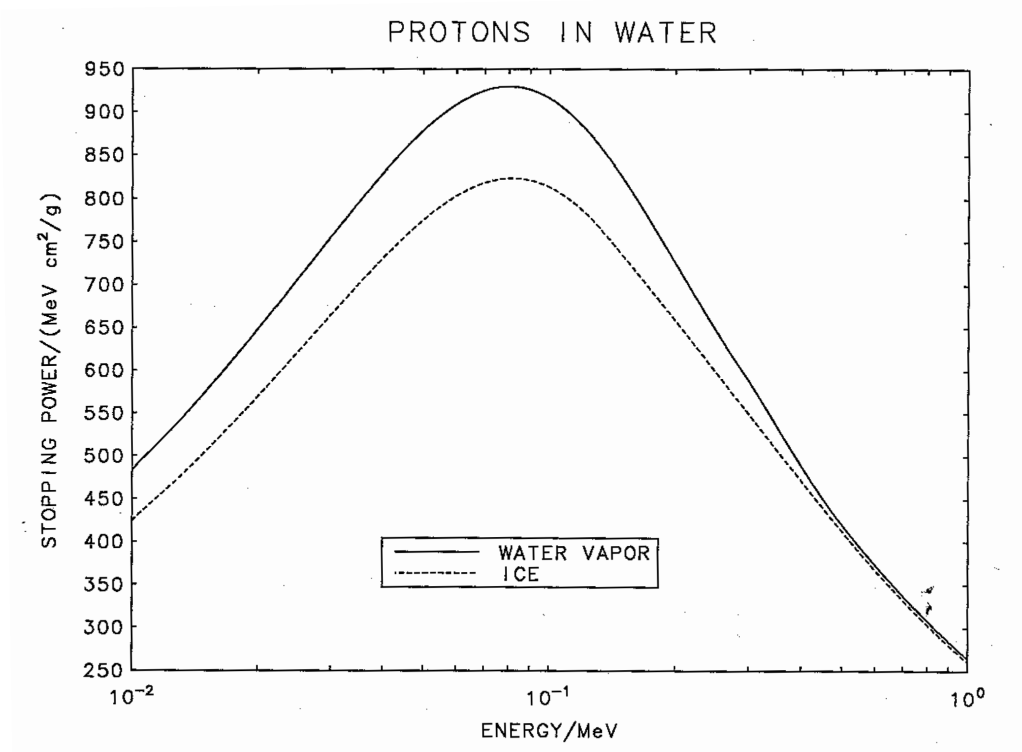
Electronic mass stopping power : Examples



Protons incident on different media

Influence of the phase

- For large energies → influence of the density correction → large correction for solids and weak correction for gases
- For small energies → influence of chemical and intermolecular bounding → modification of the value of *I* (example: liquid water: *I* = 75.0 eV and gaseous water: *I* = 71.6 eV)



Range of charged particles (1)

- Charged particles lose their energy in matter → they travel a certain distance in matter → this distance is variable because of aleatory energy losses and deviations (straggling) → different ranges have to be defined:
  - The range R of a charged particle of energy E in a medium is the mean value $\langle\ l\ \rangle$ of the length l of its trajectory as it slows down to rest (we do not take into account thermal motion)
  - The projected range R_p of a charged particle of energy E in a medium is the mean value of its penetration depth $\langle\ d\ \rangle$ along the initial direction of the particle
- $R_p < R$ due to the sinuous character of trajectories → definition of the detour factor = $R_P/R_{CSDA} < 1$

Range of charged particles (2)

- In CSDA approximation →

$$R_{CSDA} = \int_0^E \frac{dE'}{NS(E')}$$

- By replacing *S* by the Bethe expression (non-relativistic → *dE = Mvdv*) →

$$R_{CSDA} \propto \int_0^v \frac{v^3 dv}{L(v)}$$

- By neglecting the dependency into the velocity for the stopping number →

$$R_{CSDA} \propto v^4 \propto E^2$$

Range of charged particles (3)

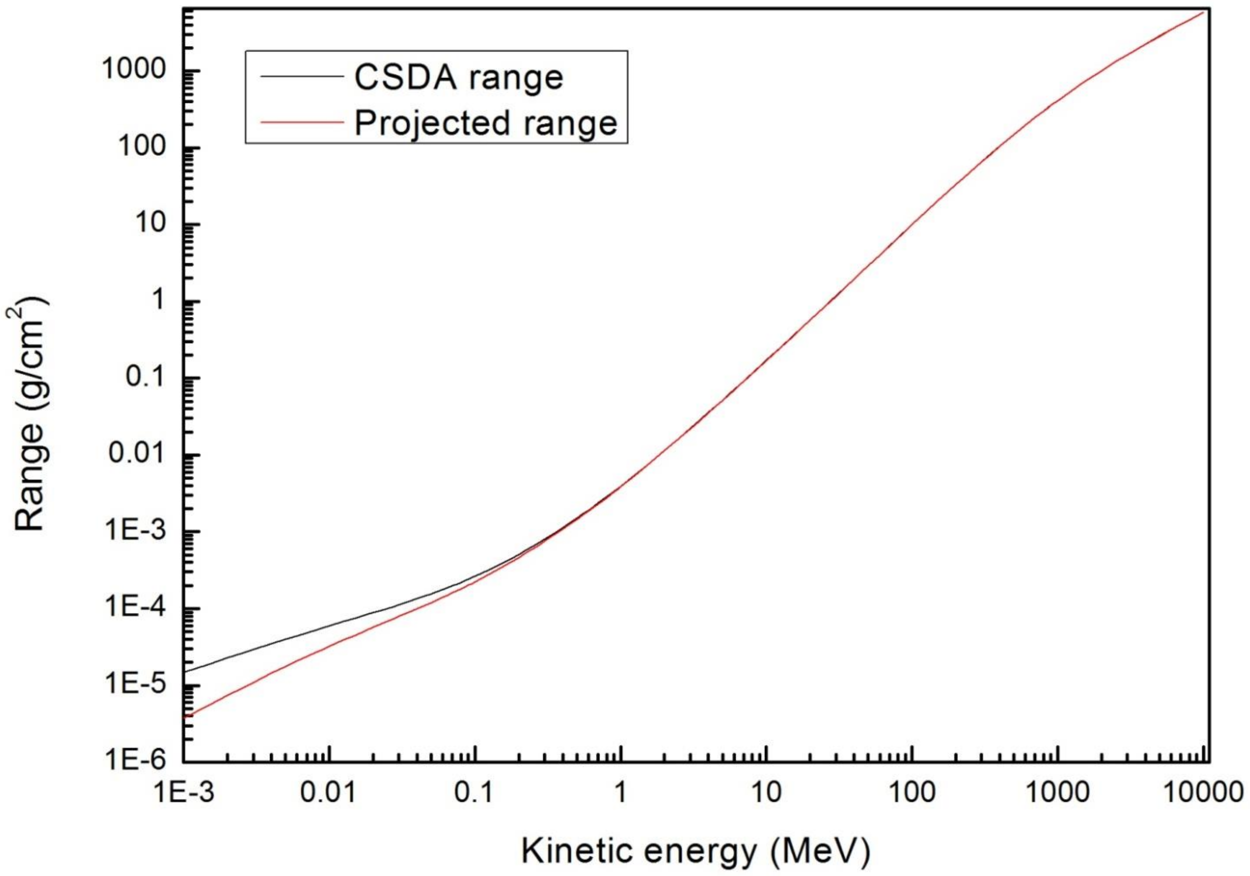
- In reality → the equation of Bethe (or Bethe-Bloch) is not valid for small velocities → but before to stop small velocities have to be considered

- We consider the empiric equation →

$$\rho R_{CSDA} = \frac{E^{1.77}}{415} + \frac{1}{670}$$

Range of charged particles: Example

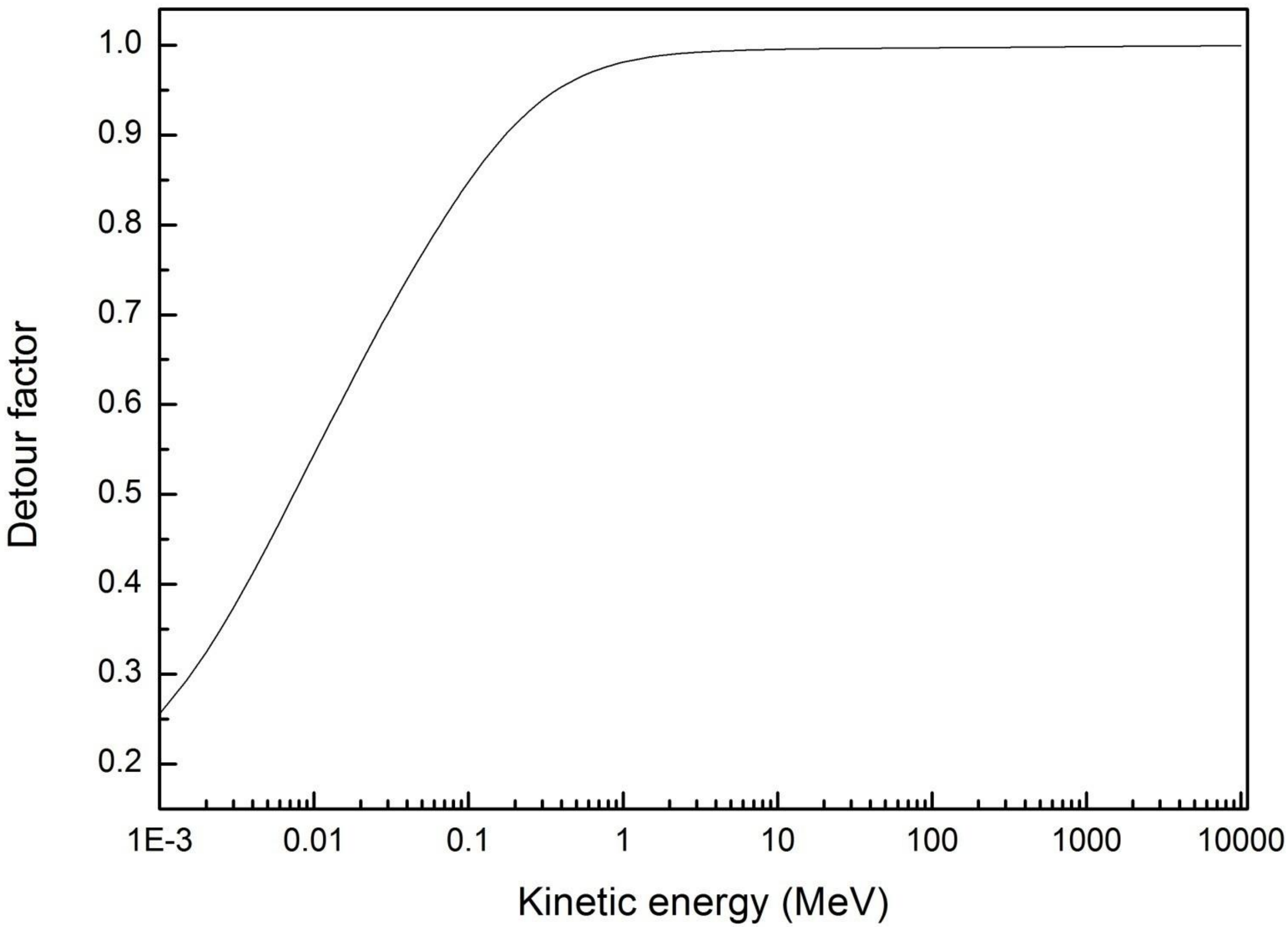
Incident proton on aluminium (ρ =2.70 g/cm^3)



http://www.nist.gov/pml/data/star/index.cfm

Detour factor

Incident proton on aluminium



Range approximations

$$S_e = \frac{4\pi r_e^2 mc^2}{\beta^2} Z z^2 L(\beta)$$

- NS(E) $\propto$ 1/E
- NS(E)/z^2 only depends on v → if we have particle of mass M_i and charge z_i:

$$NS(E) = -\frac{dE}{dx} \Rightarrow -\frac{M_i}{z_i^2}\frac{dv^2}{dx} \propto v^{-2}$$

- For 2 particles (M_1,z_1) and (M_2,z_2) of same velocity:

$$\frac{R^1_{CSDA}}{R^2_{CSDA}} = \frac{M_1 z_2^2}{M_2 z_1^2}$$

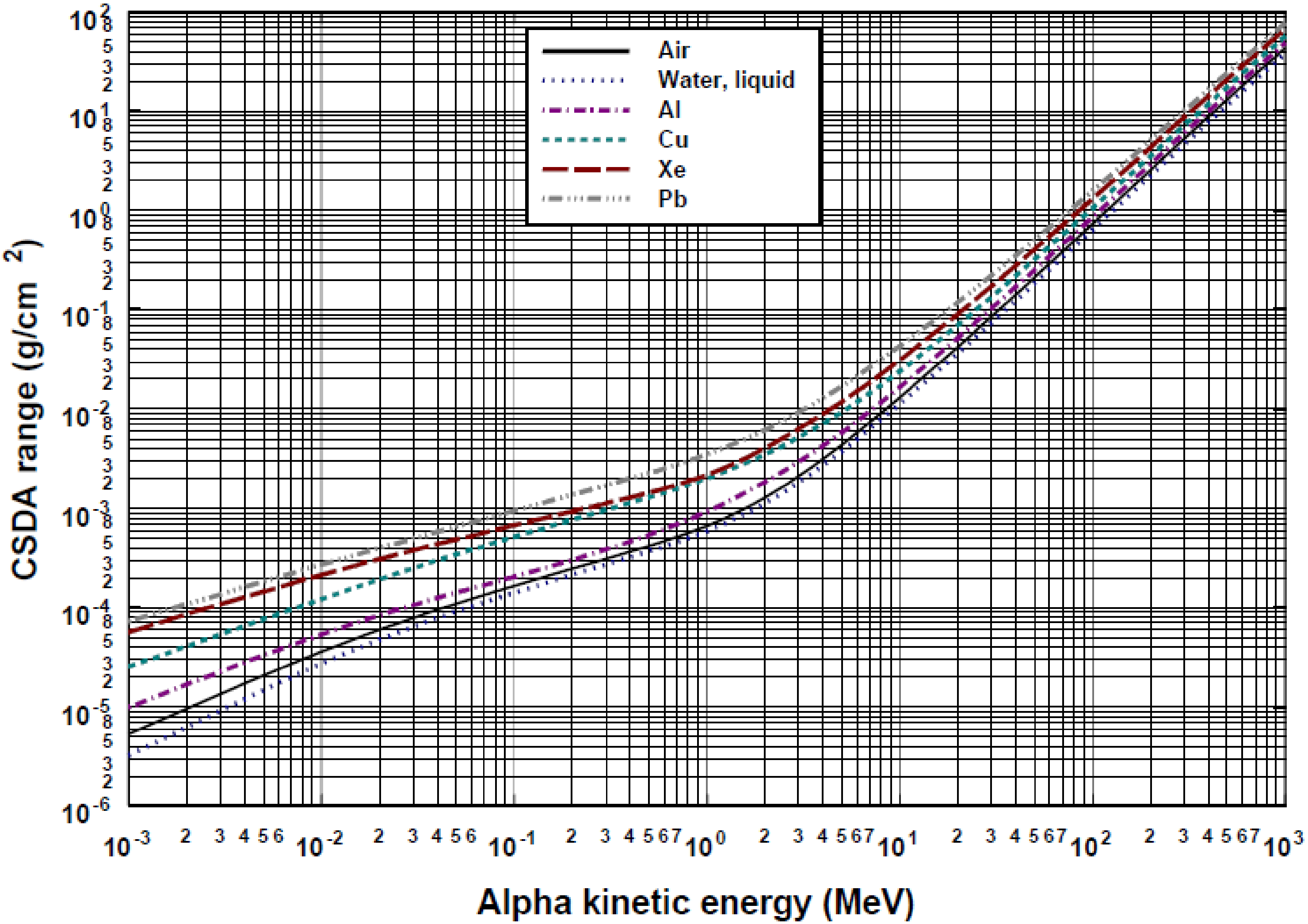
Same range for proton and α of same velocity

Examples of CSDA ranges (1)

- 5.5 MeV α in air: R_{CSDA}= 4.2 cm
- 4.0 MeV α in air: R_{CSDA}= 2.6 cm
- 5.5 MeV α in aluminium: R_{CSDA}= 2.5 10^{-3} cm
- 1 MeV proton in air: R_{CSDA}= 2.4 cm
- 4 MeV proton in air: R_{CSDA}= 23.6 cm
- 5.5 MeV proton in aluminium: R_{CSDA}= 2.3 10^{-2} cm

http://www.nist.gov/pml/data/star/index.cfm

Examples of CSDA ranges (2)



α incident on various media

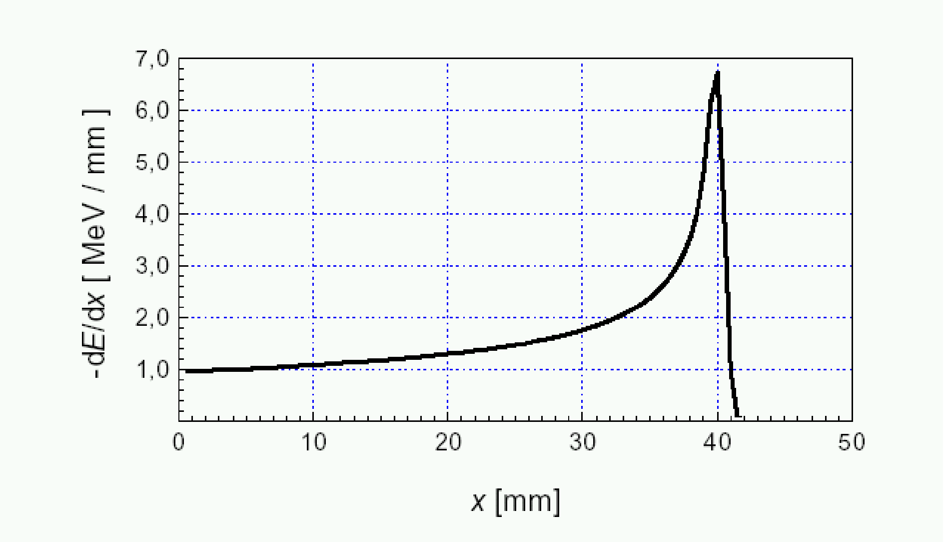
Bragg curve

- We consider a semi-infinite medium and a beam of identical parallel charged particles with same E → they stop after travelling the distance R_{CSDA}
- The Bragg curve gives the dose (mean deposited energy per mass unit of the target) as a function of the depth
- At depth x, the particle has to cover a distance $d = R_{CSDA} - x$
- The dose $D \propto S \propto 1/v^2 \rightarrow R_{CSDA} \propto v^4$

$$\Rightarrow \quad D \propto \frac{1}{\sqrt{d}} = \frac{1}{\sqrt{R_{CSDA} - x}}$$

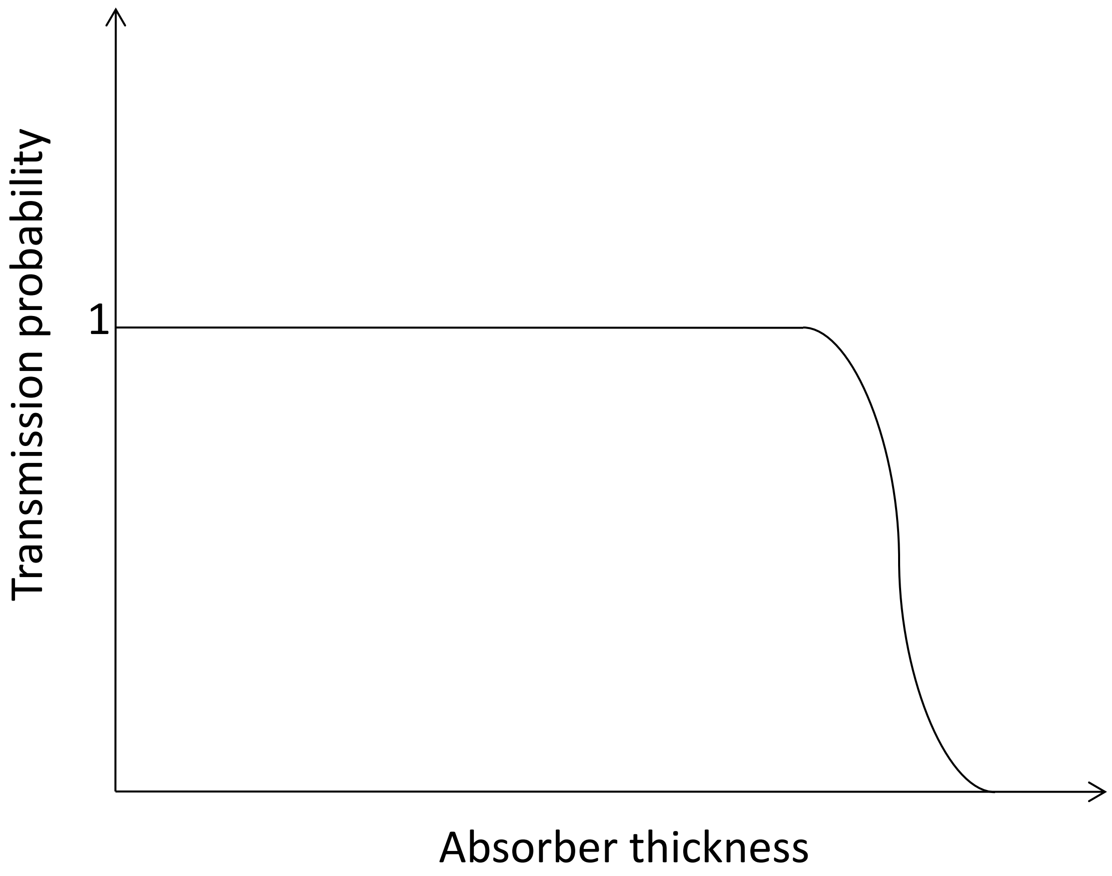
Example of Bragg curve

- Protons of 700 MeV in water →



- Applications: protontherapy or hadrontherapy

Transmission of ions



Strong nuclear interactions

- If ion comes very close to target nucleus → strong nuclear interaction becomes possible → the target nucleus will be broken up
- One particular case: the collision of a high-energy proton with a very heavy nucleus with thus more neutrons than protons (lead: 82 protons and ≈125 neutrons) → the fragments will quickly expel their excess neutrons → production of a large number of secondary neutrons (proton of 1 GeV → on average 25 neutrons in lead)
- This process of neutrons production is called spallation → efficient way to produce neutrons
- All fragments interact with matter