Ionization

Ionization

The basic mechanism is an inelastic collision of the moving charged particle with the atomic electrons of the material, ejecting off an electron from the atom :

$$p + atom \rightarrow p + atom^{+} + e^{-}$$

In each individual collision, the energy transfered to the electron is small. But the total number of collisions is large, and we can well define the average energy loss per (macroscopic) unit path length.

Mean energy loss and energetic δ-rays

$$\frac{d\sigma(Z,E,T)}{dT}$$

is the differential cross-section per atom for the ejection of an electron with kinetic energy T by an incident charged particle of total energy E moving in a material of density ρ.

One may wish to take into account separately the high-energy knock-on electrons produced above a given threshold T_{cut} (miss detection, explicit simulation ...).

$T_{cut} \gg I$ (mean excitation energy in the material).
$T_{cut} > 1$ keV in Geant4

Below this threshold, the soft knock-on electrons are counted only as continuous energy lost by the incident particle.

Above it, they are explicitly generated. Those electrons must be excluded from the mean continuous energy loss count.

The mean rate of the energy lost by the incident particle due to the soft δ-rays is :

$$\frac{dE_{soft}(E,T_{cut})}{dx} = n_{at} \cdot \int_0^{T_{cut}} \frac{d\sigma(Z,E,T)}{dT} T \, dT \qquad (1)$$

n_{at} : nb of atoms per volume in the matter.

The total cross-section per atom for the ejection of an electron of energy $T > T_{cut}$ is :

$$\sigma(Z,E,T_{cut}) = \int_{T_{cut}}^{T_{max}} \frac{d\sigma(Z,E,T)}{dT} \, dT \qquad (2)$$

where T_{max} is the maximum energy transferable to the free electron.

Mean rate of energy loss by heavy particles

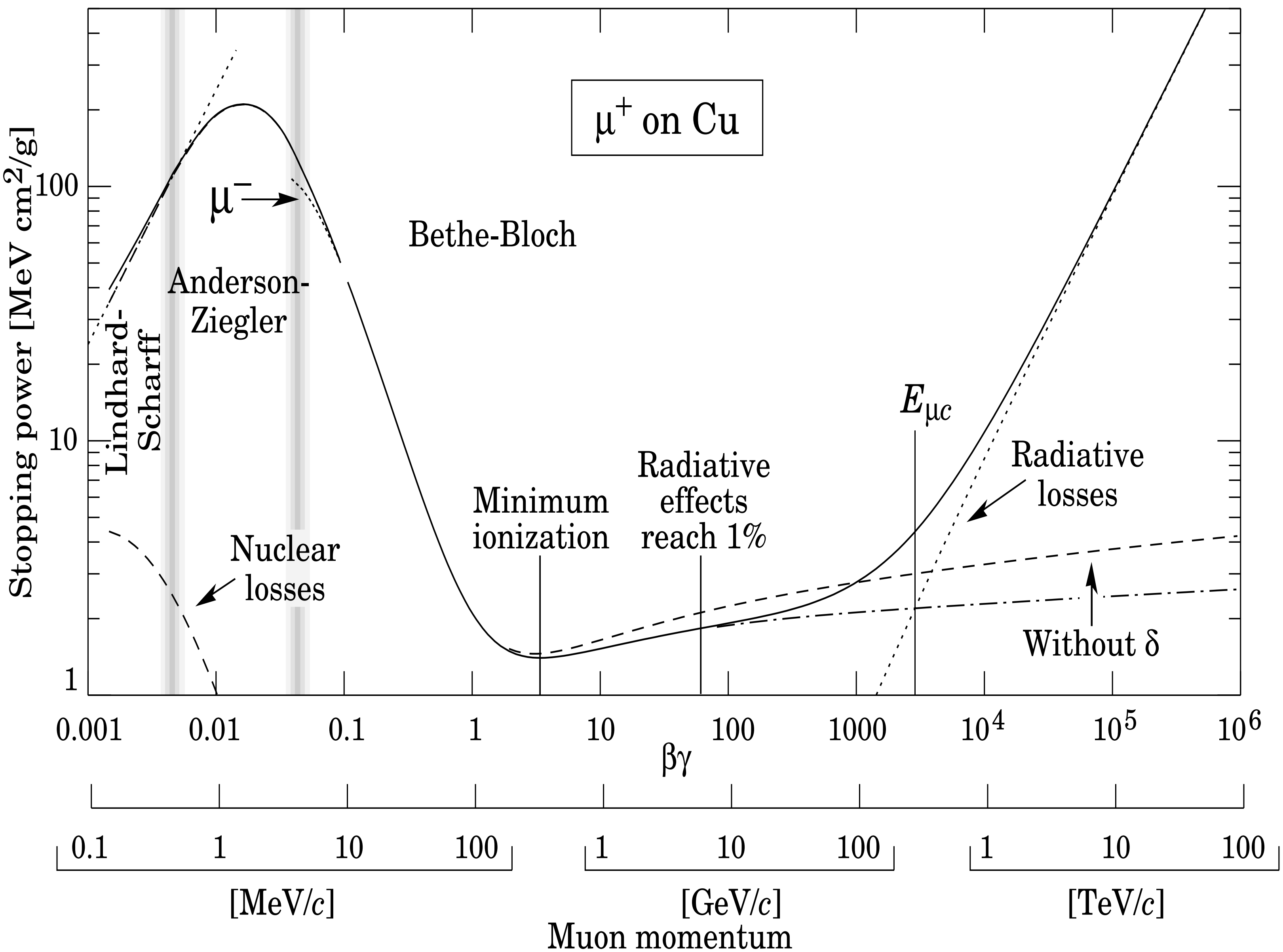
The integration of equation 1 leads to the well known Bethe-Bloch truncated energy loss formula [PDG] :

$$\left.\frac{dE}{dx}\right]_{T<T_{cut}} = 2\pi r_e^2 mc^2 n_{el} \frac{(z_p)^2}{\beta^2} \times \left[\ln\left(\frac{2mc^2\beta^2\gamma^2 T_{up}}{I^2}\right) - \beta^2\left(1+\frac{T_{up}}{T_{max}}\right) - \delta - \frac{2C_e}{Z}\right]$$

where

r_e	classical electron radius: $e^2/(4\pi\epsilon_0 mc^2)$
mc^2	energy-mass of electron
n_{el}	electrons density in the material
z_p	charge of the incident particle
T_{up}	$\min(T_{cut}, T_{max})$
I	mean excitation energy in the material
δ	density effect function
C_e	shell correction function

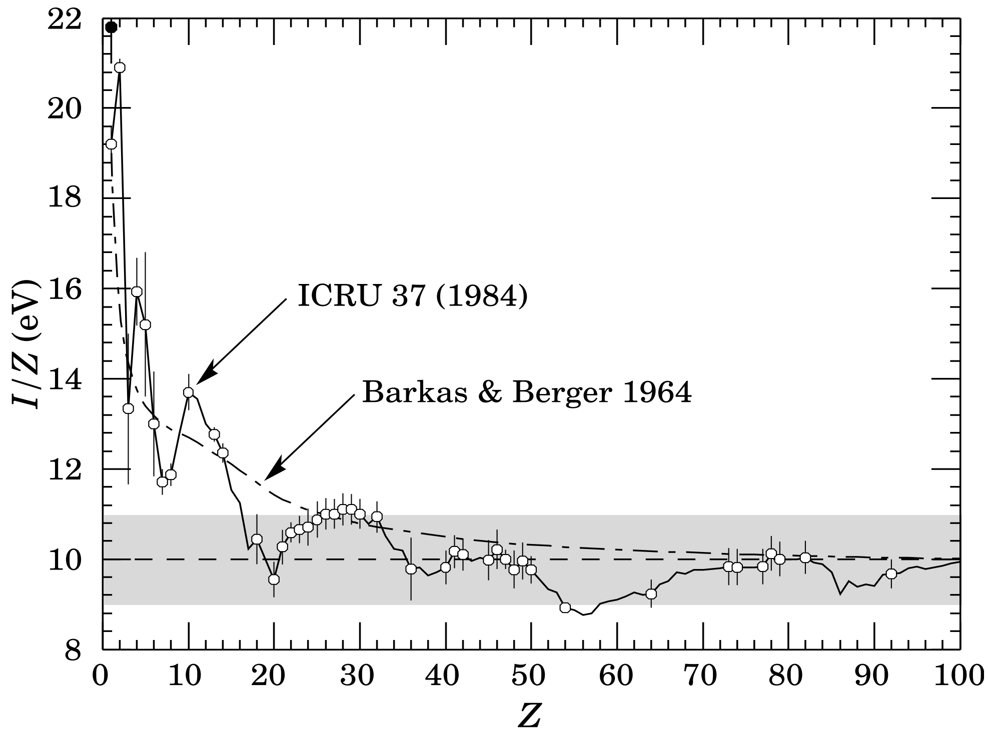
$$n_{el} = Z\, n_{at} = Z\, \frac{\mathcal{N}_{av}\rho}{A} \qquad T_{max} = \frac{2mc^2(\gamma^2-1)}{1+2\gamma m/M+(m/M)^2}$$


μ+ on Cu
μ−
Bethe-Bloch
Anderson-
Ziegler
Lindhard-
Scharff
Nuclear
losses
Minimum
ionization
Radiative
effects
reach 1%
Eμc
Radiative
losses
Without δ
Stopping power [MeV cm2/g]
100
10
1
0.001
0.01
0.1
1
10
100
1000
10^4
10^5
10^6
βγ
0.1
1
10
100
1
10
100
1
10
100
[MeV/c]
[GeV/c]
[TeV/c]
Muon momentum

mean excitation energy

There exists a variety of phenomenological approximations for I, the simplest being $I = 10eV \times Z$

In Geant4 we have tabulated the recommended values in [ICRU84].



the density effect

δ is a correction term which takes into account of the reduction in energy loss due to the so-called density effect. This becomes important at high energy because media have a tendency to become polarised as the incident particle velocity increases. As a consequence, the atoms in a medium can no longer be considered as isolated. To correct for this effect the formulation of Sternheimer [Ster71] is generally used.

the shell correction

$2C_e/Z$ is a so-called *shell correction term* which accounts for the fact that, under certain conditions, the probability of collision with the electrons of the inner atomic shells (K, L, etc.) is negligible. The semi-empirical formula used in GEANT4, applicable to all materials, is due to Barkas [Bark62]:

$$C_e(I, \beta\gamma) = \frac{a(I)}{(\beta\gamma)^2} + \frac{b(I)}{(\beta\gamma)^4} + \frac{c(I)}{(\beta\gamma)^6}$$

low energies

The mean energy loss can be described by the Bethe-Bloch formula only if the projectile velocity is larger than that of orbital electrons. In the low-energy region where this is not verified, a different kind of parameterisation must be used.
For instance:

- Andersen and Ziegler [Ziegl77] for $0.01 < \beta < 0.05$
- Lindhard [Lind63] for $\beta < 0.01$

See ICRU Report 49 [ICRU93] for a detailed discussion of low-energy corrections.

low energies

in `G4hIonisation`, a simple parametrisation gives the energy loss as a function of $\tau = (T/M_{proton}c^2)$:

$$dE/dx = n_{el} \cdot (A\sqrt{\tau} + B\tau) \quad \text{for} \quad \tau \leq \tau_0$$
$$dE/dx = n_{el} \cdot C/\sqrt{\tau} \quad \text{for} \quad \tau \in [\tau_0,\ \tau_1]$$

The parameters A, B, C are such that dE/dx is a continuous function of the kinetic energy T at τ_0 and τ_1.

Above T_1 the truncated Bethe-Bloch formula is used.

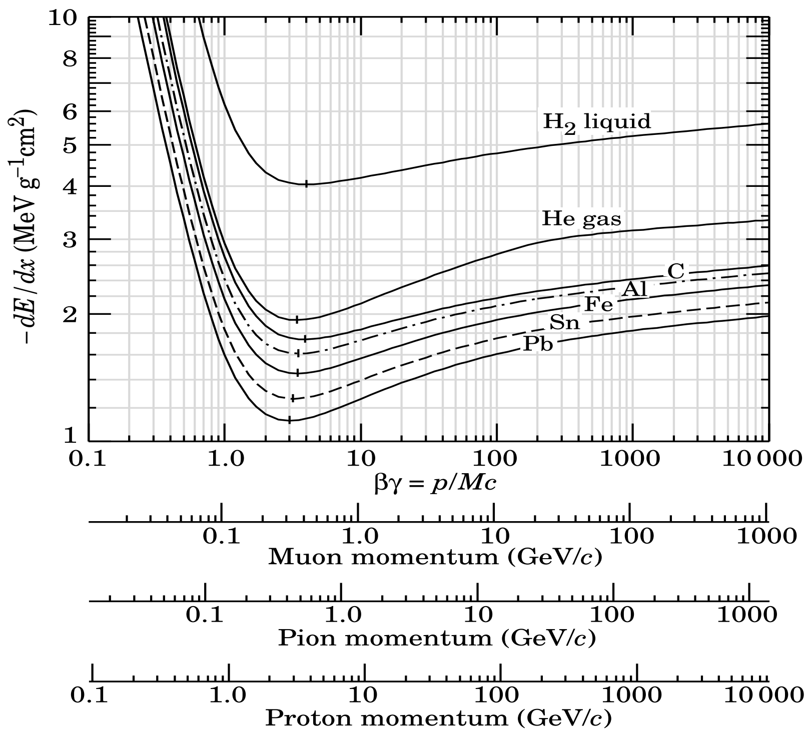
PhysicsTables

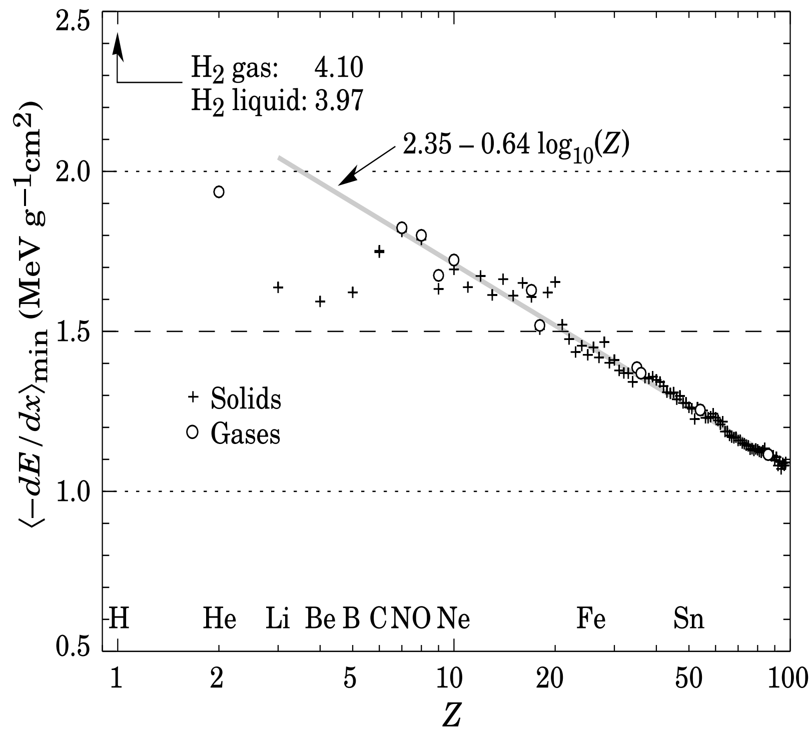
At initialization stage, the function `BuildPhysicsTables()` computes and tabulates the dE/dx due to the soft δ-rays, as a function on energy, and for all materials.

The dE/dx of charged hadrons is obtained from that of proton (or antiproton) by calculating the kinetic energy of a proton with the same β, and using this value to interpolate the proton tables.

$$T_{proton} = \frac{M_{proton}}{M}\, T$$

minimum ionization



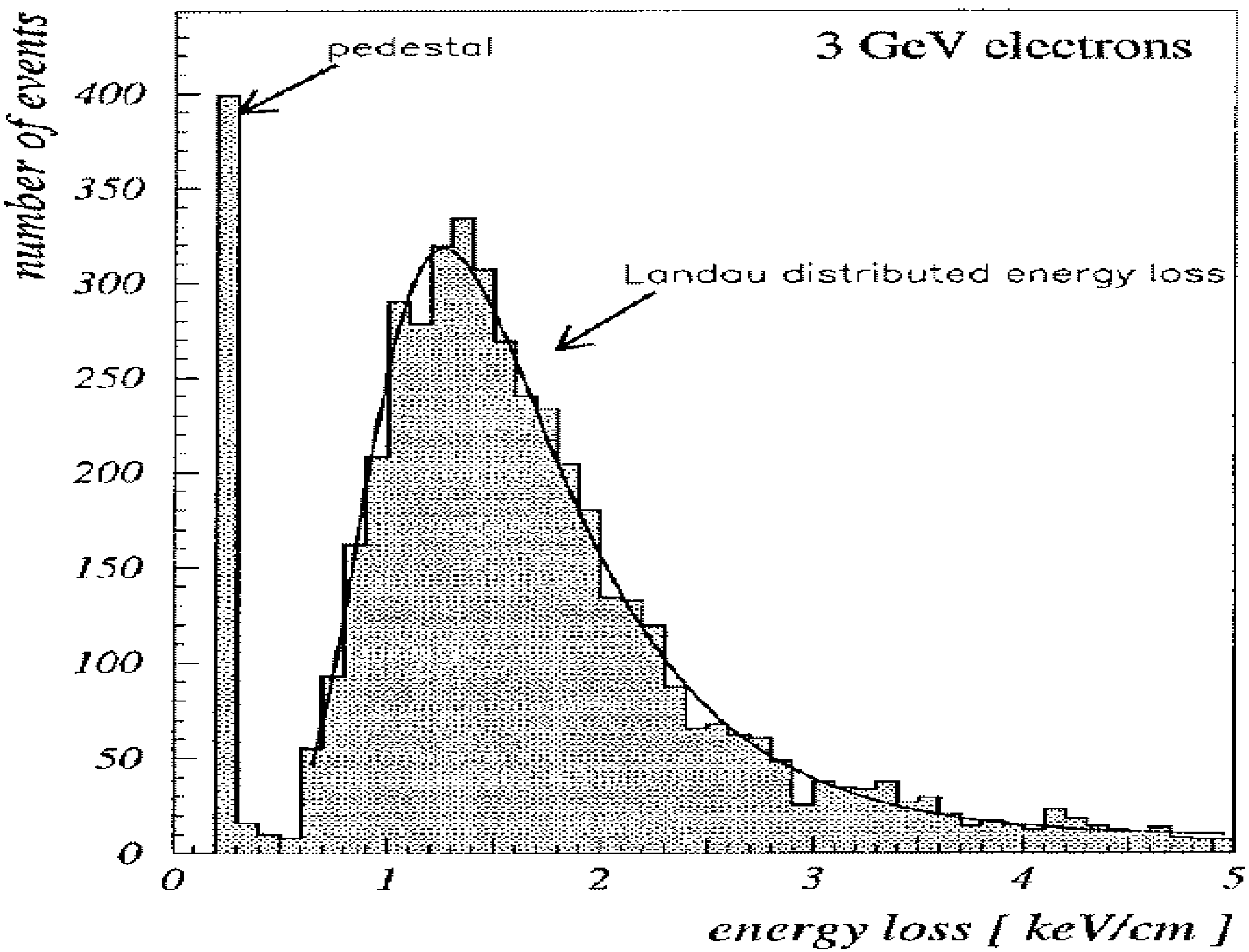


Fluctuations in energy loss

$\langle \Delta E \rangle = (dE/dx).\Delta x$ gives only the average energy loss by ionization. There are fluctuations. Depending of the amount of matter in Δx the distribution of ΔE can be strongly asymmetric ($\rightarrow$ the Landau tail).

The large fluctuations are due to a small number of collisions with large energy transfers.

The figure shows the energy loss distribution of 3 GeV electrons in 5 mm of an Ar/CH4 gas mixture [Affh98].



Energy loss fluctuations : the models in Geant

The straggling is partially taken into account by the simulation of energy loss by the production of δ-electrons with energy $T > T_{cut}$. However continuous energy loss also has fluctuations.

Two different models of fluctuations are applied depending on the value of the parameter κ which is the lower limit of the number of potential interactions of the particle in the step:

$$\kappa = \frac{\Delta E}{T_{cut}}$$

where ΔE is the mean continuous energy loss in a track segment of length Δx.

Energy loss fluctuations : Gaussian regime

For $\kappa \geq 10$ and if T_{max} is not too big ($T_{max} \leq 2T_{cut}$) the straggling function approaches a Gaussian distribution with Bohr's variance [ICRU93]:

$$\Omega^2 = 2\pi r_e^2 \; m_e c^2 \; n_{el} \; \frac{Z_h^2}{\beta^2} \; \Delta x \; T_{cut} \left(1 - \frac{\beta^2}{2}\right)$$

(Z_h is the charge of the incident particle in units of positron charge.)

Energy loss fluctuations : Urban model

For $\kappa < 10$.
It is based on a rather simple model of the particle-atom interaction.

The atoms are assumed to have only two energy levels E_1 and E_2.

The particle-atom interaction can be :

- an excitation with energy loss E_1 or E_2
- an ionization with energy loss distribution $g(E) \sim 1/E^2$, with $E \in [E_0,\ T_{up}]$.

$$\int_{E_0}^{T_{up}} g(E)\ dE = 1 \Longrightarrow g(E) = \frac{E_0 T_{up}}{T_{up} - E_0} \frac{1}{E^2}$$

The macroscopic cross section for excitation $(i = 1, 2)$ is :

$$\Sigma_i = \left\langle \frac{dE}{dx} \right\rangle \; \frac{f_i}{E_i} \; \frac{\ln[2mc^2 \; (\beta\gamma)^2/E_i] - \beta^2}{\ln[2mc^2 \; (\beta\gamma)^2/I] - \beta^2} \; (1 - r)$$

I = mean excitation energy

$E_i, \; f_i$ = energy levels and oscillator strengths of the atom

r is a model parameter.

f_i and E_i must satisfy the sum rules [Bichs88] :

$$f_1 + f_2 = 1$$

$$f_1 \cdot \ln E_1 + f_2 \cdot \ln E_2 = \ln I$$

For ionization :

$$\Sigma_3 = \left\langle \frac{dE}{dx} \right\rangle \; \frac{T_{up} - E_0}{E_0 T_{up} \ln(\frac{T_{up}}{E_0})} \; r$$

$E_0 =$ ionization energy of the atom

$T_{up} = \min(T_{max}, T_{cut})$

In a step of length Δx the nb of collisions n_i, ($i = 1, 2$ for excitation, 3 for ionization) follows a Poisson distribution with :

$$\langle n_i \rangle = \Delta x \; \Sigma_i$$

The mean energy loss in a step is the sum of the excitation and ionization contributions :

$$\left\langle \frac{dE}{dx} \right\rangle \cdot \Delta x = \left\{ \Sigma_1 E_1 + \Sigma_2 E_2 + \int_{E_0}^{T_{up}} E g(E) dE \right\} \Delta x$$

E_2 is approximately the K-shell energy of atoms : $E_2 = 10$ eV Z^2
$E_0 = 10$ eV
$Z f_2 = 2$ is the number of K-shell electrons.
f_1 and E_1 can be obtained from the sum rules.

The parameter r is the only variable in the model which can be tuned. This parameter determines the relative contribution of ionization and excitation to the energy loss.

Its value has been parametrized from comparison of simulated energy loss distributions to experimental data :

$$r = 0.03 + 0.23 \ln \left[\ln \left(\frac{T_{up}}{I} \right) \right]$$

Sample the energy loss : the loss due to the excitation is

$$\Delta E_{exc} = n_1 E_1 + n_2 E_2$$

where n_1 and n_2 are sampled from Poisson distribution.

The energy loss due to the ionization can be generated from the distribution $g(E)$ by the inverse transformation method. Then, the contribution from the ionization will be :

$$\Delta E_{ion} = \sum_{j=1}^{n3} \frac{E_0}{1 - u_j \frac{T_{up} - E_0}{T_{up}}}$$

n_3 is the nb of ionizations sampled from Poisson distribution,
u_j is uniform $\in [0,\ 1]$.

The total energy loss in a step Δx is $\Delta E = \Delta E_{exc} + \Delta E_{ion}$
The energy loss fluctuation comes from the fluctuations of the collision numbers n_i

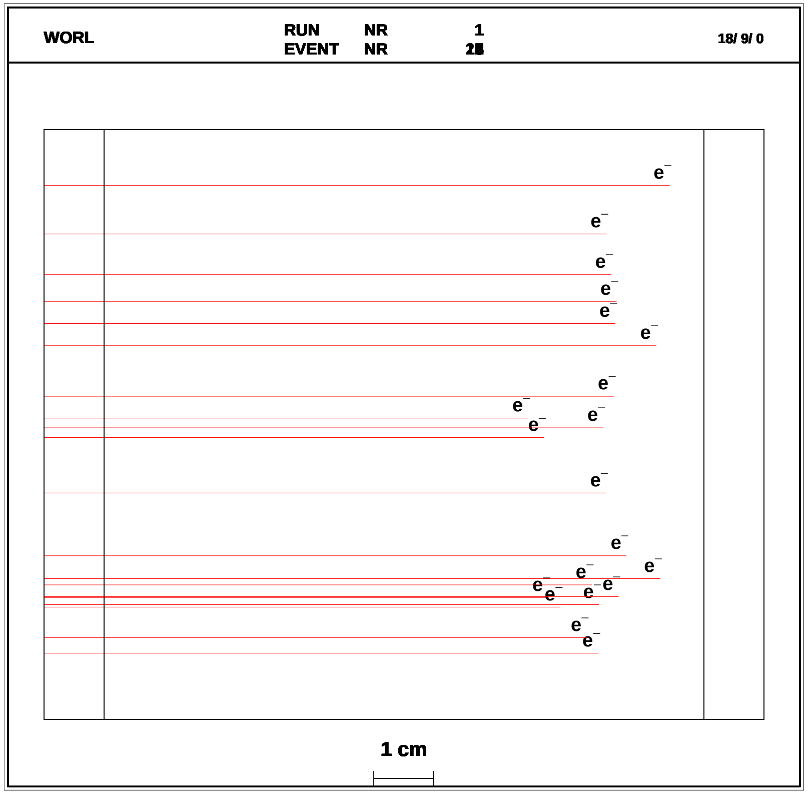
This simple model of the energy loss fluctuations is rather fast and it can be used for any thickness of the materials, and for any T_{cut}.

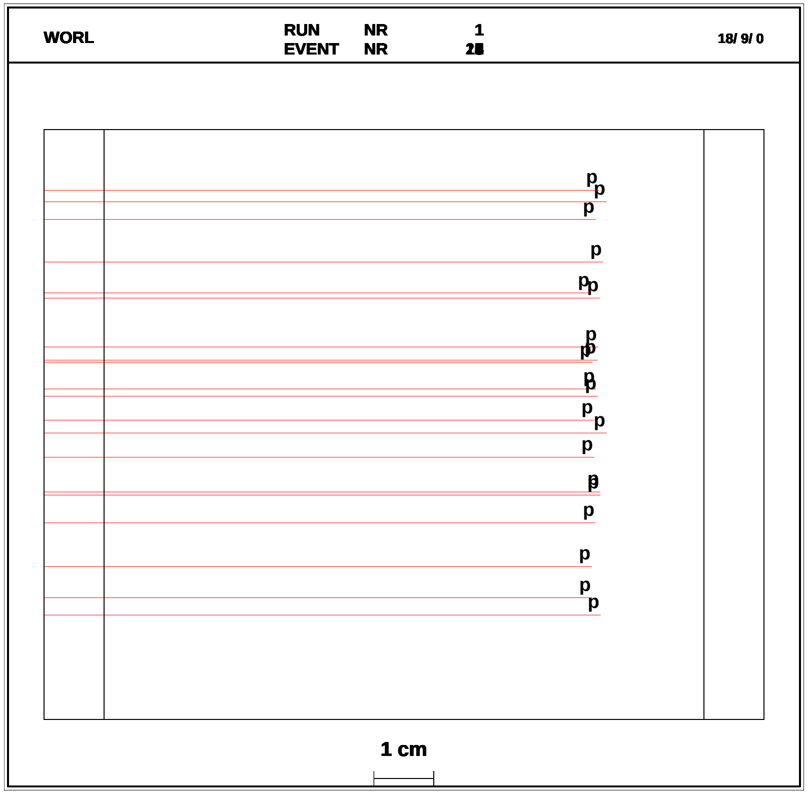
This has been proved performing many simulations and comparing the results with experimental data, see e.g [Urban95].

Approaching the limit of the validity of Landau's theory, the loss distribution approaches smoothly the Landau form.

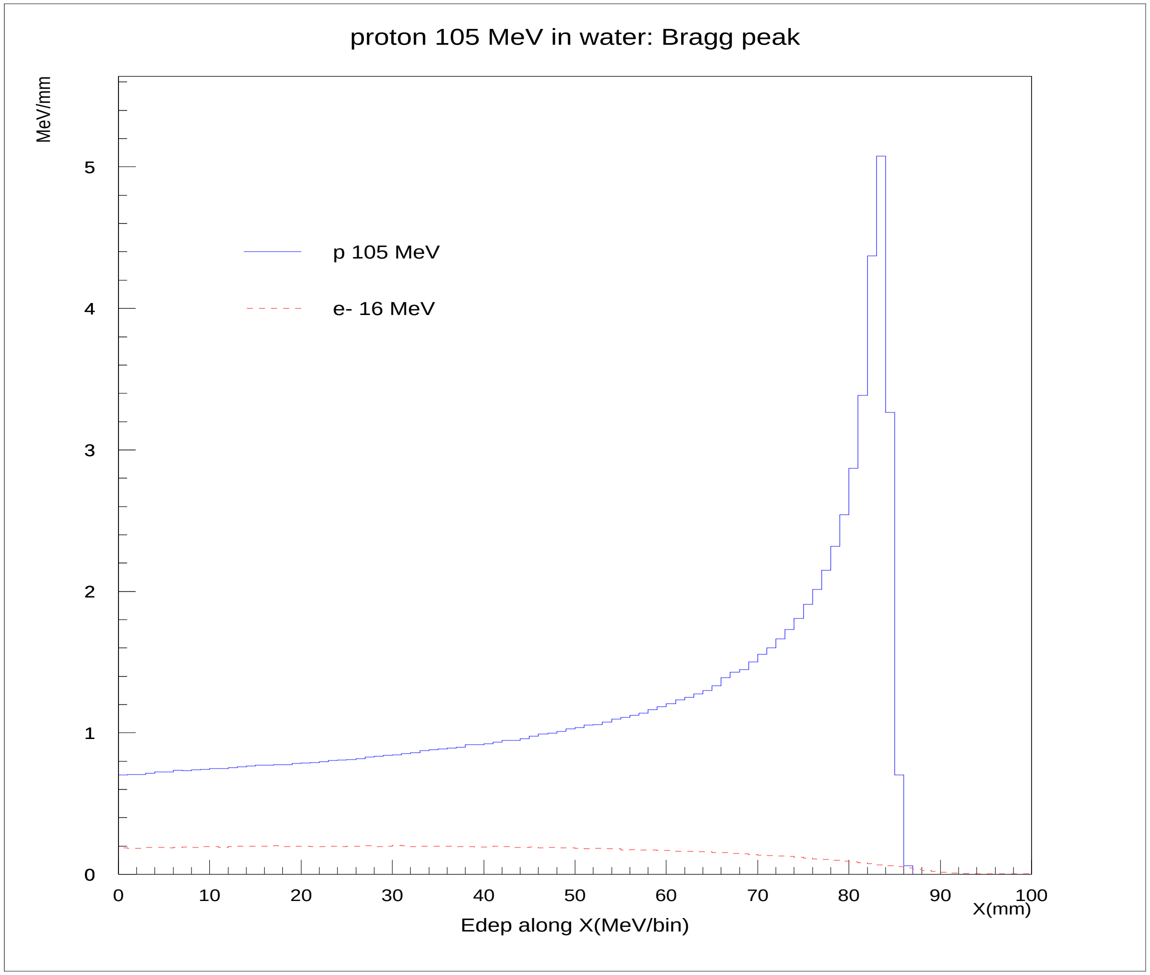
Fluctuations on ΔE lead to fluctuations on the actual range (straggling).

penetration of e^- (16 MeV) and proton (105 MeV) in 10 cm of water.





Bragg curve. More energy per unit length are deposit towards the end of trajectory rather at its beginning.



Energetic δ rays

The differential cross-section per atom for producing an electron of kinetic energy T, with $I \ll T_{cut} \leq T \leq T_{max}$, can be written :

$$\frac{d\sigma}{dT} = 2\pi r_e^2 mc^2 Z \frac{z_p^2}{\beta^2} \frac{1}{T^2} \left[1 - \beta^2 \frac{T}{T_{max}} + \frac{T^2}{2E^2} \right]$$

(the last term for spin 1/2 only).

The integration of equation(2) gives :

$$\begin{aligned} \sigma(Z,E,T_{cut}) &= \frac{2\pi r_e^2 Z z_p^2}{\beta^2} \left[\left(\frac{1}{T_{cut}} - \frac{1}{T_{max}} \right) - \frac{\beta^2}{T_{max}} \ln \frac{T_{max}}{T_{cut}} \right. \\ & \left. + \frac{T_{max} - T_{cut}}{2E^2} \right] \end{aligned}$$

(the last term for spin 1/2 only).

Mean free path

$$\lambda(E, T_{cut}) = \left(\sum_i n_{ati} \cdot \sigma(Z_i, E, T_{cut}) \right)^{-1}$$

n_{ati} : nb of atoms per volume of the i^{th} element in the material.

At initialization stage, the function `BuildPhysicsTables()` computes and tabulates :

- meanFreePath for all materials

sample the energy of the δ-ray

Apart from the normalisation, the cross-section can be factorised :

$$\frac{d\sigma}{dT} = f(T)\, g(T) \quad with \quad T \in [T_{cut},\ T_{max}]$$

with :

$$f(T) = \left(\frac{1}{T_{cut}} - \frac{1}{T_{max}}\right)\frac{1}{T^2}$$

$$g(T) = 1 - \beta^2\frac{T}{T_{max}} + \frac{T^2}{2E^2}$$

(the last term in $g(T)$ for spin 1/2 only).

The energy T is obtained by :

1. sample T from $f(T)$
2. accept/reject the sampled T with a probability $g(T)$.

compute the final kinematic

The function `AlongStepDoIt()` computes the energy lost by the ionizing particle, along its step.

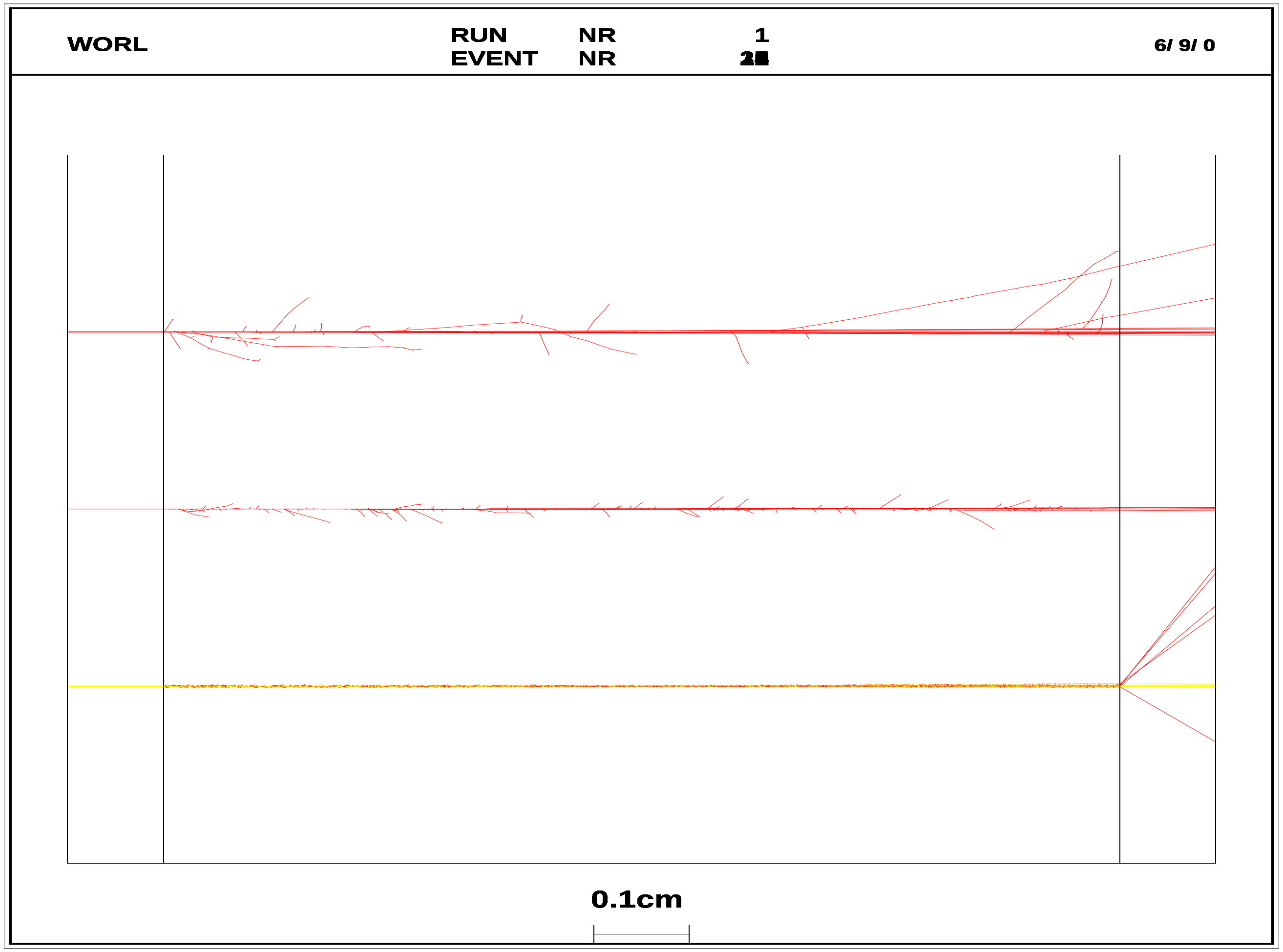
The function `PostStepDoIt()` samples the energy of the knock-on electron.

Then, the direction of the scattered electron is generated with respect to the direction of the incident particle :
θ is calculated from the energy momentum conservation.
ϕ is generated isotropically.

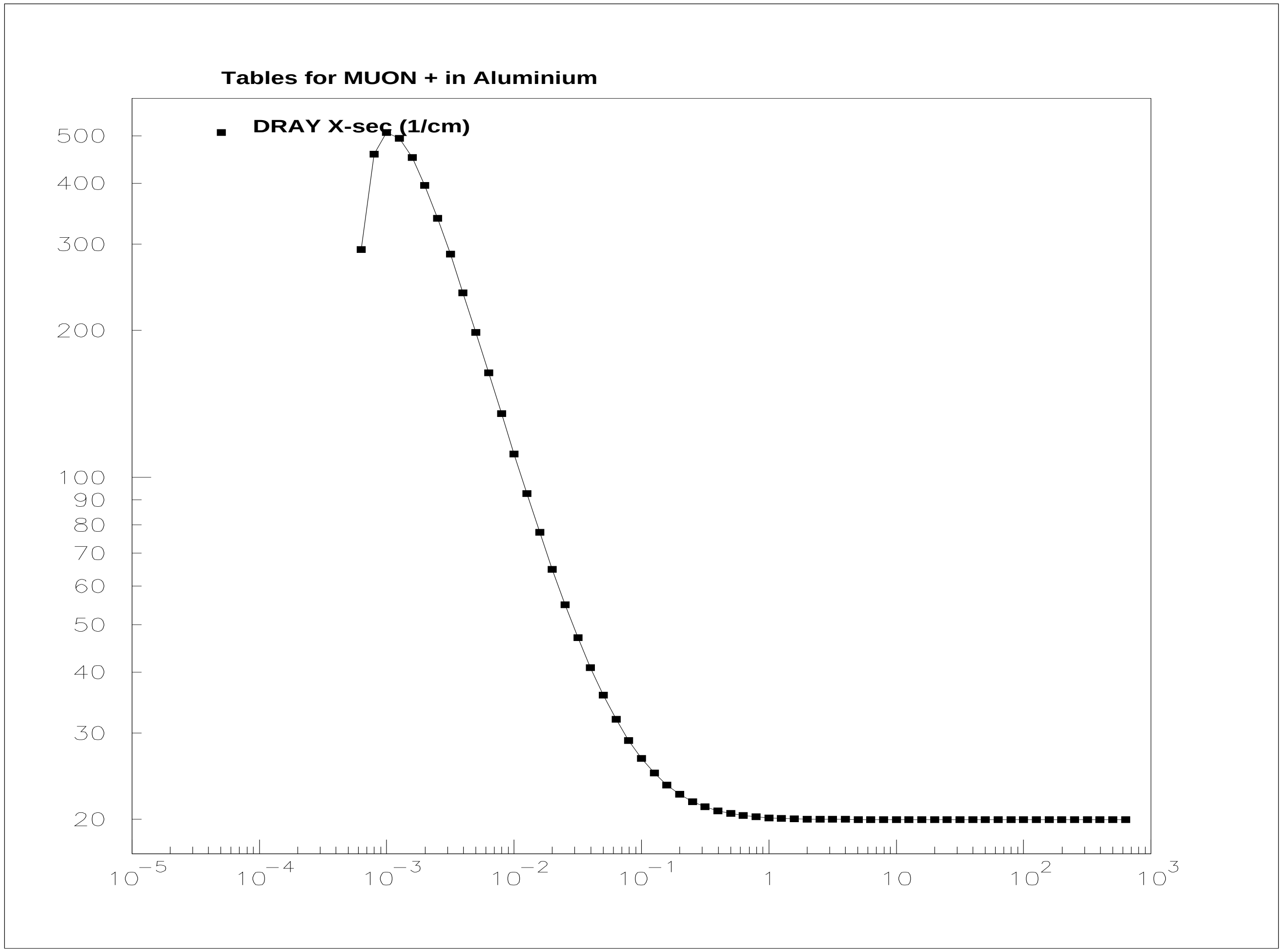
This information is used to calculate the energy and momentum of both scattered particles and to transform them into the *global* coordinate system.

delta rays

200 MeV electrons, protons, alphas in 1 cm of Aluminium



muon : number of δ-rays per cm in Aluminium



muon kinetic energy (GeV)

Incident electrons and positrons

For incident $e^{-/+}$ the Bethe Bloch formula must be modified because of the mass and identity of particles (for e^-).

One use the Moller or Bhabha cross sections [Mess70] and the Berger-Seltzer dE/dx formula [ICRU84, Selt84].

truncated Berger-Seltzer dE/dx formula

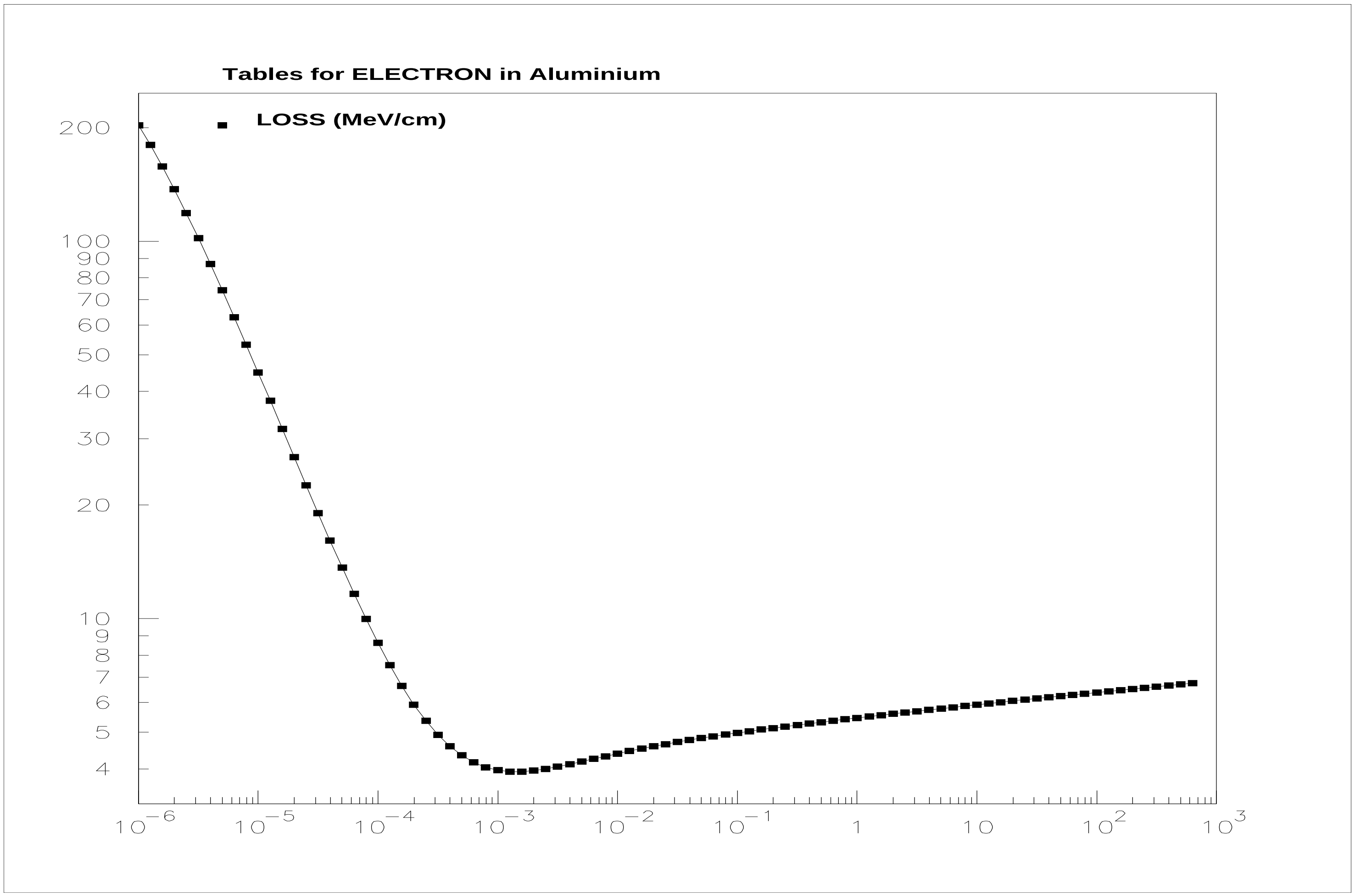
$$\left.\frac{dE}{dx}\right]_{T<T_{cut}} = 2\pi r_e^2 mc^2 n_{el} \frac{1}{\beta^2} \times \left[\ln\left(\frac{2(\gamma+1)}{(I/mc^2)^2}\right) + F^{\pm}(\gamma-1,\tau_{up}) - \delta\right]$$

where

T_{cut}	energy cut for $\delta - ray$
τ_c	T_{cut}/mc^2
τ_{max}	maximum energy transfer: $\gamma - 1$ for e^+, $(\gamma-1)/2$ for e^-
τ_{up}	$\min(\tau_c, \tau_{max})$

The functions $F^{\pm}$ are given in [Selt84].

de/dx due to ionization (Berger-Seltzer formula)



electron kinetic energy (GeV)

differential cross section per atom (for $T \gg I$)

For the electron-electron (Möller) scattering we have:

$$\frac{d\sigma}{d\epsilon} = \frac{2\pi r_e^2 Z}{\beta^2(\gamma-1)} \times \left[\frac{(\gamma-1)^2}{\gamma^2} + \frac{1}{\epsilon}\left(\frac{1}{\epsilon} - \frac{2\gamma-1}{\gamma^2}\right) + \frac{1}{1-\epsilon}\left(\frac{1}{1-\epsilon} - \frac{2\gamma-1}{\gamma^2}\right)\right]$$

and for the positron-electron (Bhabha) scattering:

$$\frac{d\sigma}{d\epsilon} = \frac{2\pi r_e^2 Z}{(\gamma-1)}\left[\frac{1}{\beta^2\epsilon^2} - \frac{B_1}{\epsilon} + B_2 - B_3\epsilon + B_4\epsilon^2\right]$$

where

$$\begin{aligned} E &= \text{energy of the incident particle} \\ \gamma &= E/mc^2 & y &= 1/(\gamma+1) \\ B_1 &= 2 - y^2 & B_2 &= (1-2y)(3+y^2) \\ B_3 &= (1-2y)^2 + (1-2y)^3 & B_4 &= (1-2y)^3 \\ \epsilon &= T/(E - mc^2) \end{aligned}$$

with T the kinematic energy of the scattered electron.

The kinematical limits for the variable ϵ are:

$$\epsilon_0 = \frac{T_{cut}}{E - mc^2} \le \epsilon \le \frac{1}{2} \quad \text{for } e^-e^- \qquad \epsilon_0 \le \epsilon \le 1 \quad \text{for } e^+e^-$$

Total cross-sections per atom

The integration of formula 2 gives the total cross-section per atom, for Möller scattering (e^-e^-) :

$$\sigma(Z,E,T_{cut}) = \frac{2\pi r_e^2 Z}{\beta^2(\gamma-1)}\left[\frac{(\gamma-1)^2}{\gamma^2}\left(\frac{1}{2}-x\right)+\frac{1}{x}-\frac{1}{1-x}\right.$$
$$\left.-\frac{2\gamma-1}{\gamma^2}\ln\frac{1-x}{x}\right]$$

and for Bhabha scattering (e^+e^-) :

$$\sigma(Z,E,T_{cut}) = \frac{2\pi r_e^2 Z}{(\gamma-1)}\left[\frac{1}{\beta^2}\left(\frac{1}{x}-1\right)+B_1\ln x+B_2(1-x)\right.$$
$$\left.-\frac{B_3}{2}(1-x^2)+\frac{B_4}{3}(1-x^3)\right]$$

where

$$
\begin{aligned}
\gamma &= E/mc^2 & B_1 &= 2 - y^2 \\
\beta^2 &= 1 - (1/\gamma^2) & B_2 &= (1 - 2y)(3 + y^2) \\
x &= T_{cut}/(E - mc^2) & B_3 &= (1 - 2y)^2 + (1 - 2y)^3 \\
y &= 1/(\gamma + 1) & B_4 &= (1 - 2y)^3
\end{aligned}
$$

sample the energy of the δ-ray

Apart from the normalisation, the cross-section are factorised as :

$$\frac{d\sigma}{d\epsilon} = f(\epsilon)\ g(\epsilon)$$

for $e^- e^-$ scattering :

$$f(\epsilon) = \frac{1}{\epsilon^2}\frac{\epsilon_0}{1-2\epsilon_0}$$

$$g(\epsilon) = \frac{4}{9\gamma^2-10\gamma+5}\left[(\gamma-1)^2\epsilon^2-(2\gamma^2+2\gamma-1)\frac{\epsilon}{1-\epsilon}+\frac{\gamma^2}{(1-\epsilon)^2}\right]$$

and for $e^+ e^-$ scattering :

$$f(\epsilon) = \frac{1}{\epsilon^2}\frac{\epsilon_0}{1-\epsilon_0}$$

$$g(\epsilon) = \frac{B_0-B_1\epsilon+B_2\epsilon^2-B_3\epsilon^3+B_4\epsilon^4}{B_0-B_1\epsilon_0+B_2\epsilon_0^2-B_3\epsilon_0^3+B_4\epsilon_0^4}$$

Here $B_0 = \gamma^2/(\gamma^2-1)$ and all the other quantities have been defined above.

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