

Sampling Algorithms for the Electron Ionization Differential Cross Section

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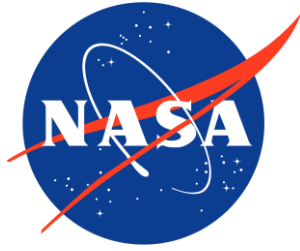
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Abstract

Monte-Carlo track structure simulation codes are widely used in radiation biophysics, dosimetry, microdosimetry, radiation chemistry, clinical radiotherapy and in space radiation risk assessment. These codes provide an accurate description of the passage of ionizing radiation in water, which is often used as a surrogate for biological tissue. Existing codes can simulate a variety of different types of radiation. One of the most important effects of ionizing radiation is the production of secondary electrons, most of them with energy below 100 eV. These secondary electrons also interact with the medium and ionize more electrons. The models of Rudd [Rudd 1990] and Seltzer [Seltzer 1988] provide useful equations of the electron ionization differential cross sections, which are commonly used in radiation transport codes to simulate energy loss happening during ionizations. In this document, efficient methods to sample electron energy loss using these cross sections are presented.

1. Introduction

Ionizing radiation creates many electrons in the irradiated medium, most of them with energies below 100 eV [Pimblott and LaVerne 2007]. Such electrons are known to produce further ionization and excitation events leading to the formation of the so-called radiation chemical spurs [Mozumder and Magee 1966]. At low energies (<20 eV), electrons can undergo resonant scattering with molecules yielding reactive radicals and molecular species, which can result in DNA breaks and oxidative damage to non-DNA molecules in biological matter [Boudaïffa et al. 2000]. High energy electrons are also very important in the study of ion track structure because they interact with many target molecules, which generate the so-called penumbra or radial extension of energetic ion tracks [Muroya et al. 2006].

The study of energetic charged particle transport through matter has produced numerous radiation transport models used in applications such as radiotherapy, accelerator beam analysis, and space radiation protection. Monte Carlo simulation codes such as RITRACKS [Plante and Cucinotta 2011] and the Geant4-DNA extension [Incerti 2010] of Geant4 [Agostinelli 2003] are Monte Carlo track structure codes of radiation transport and require random sampling of distributions describing interaction probabilities, particle emission spectra, and other physical characteristics germane to the application of interest.

In both RITRACKS and Geant4-DNA track structure simulations, the ionization of atoms in the target media by ions and electrons resulting in the liberation of secondary electrons is the dominant interaction. Rudd [Rudd 1990] developed a simple and accurate model for the energy spectrum of these secondary electrons that is used in numerous simulation codes, including RITRACKS. At higher energies (>50 keV), Seltzer's cross section model [Seltzer 1988] is used in RITRACKS. Given the high frequency of target ionizations in track structure simulations, it is critical that sampling of the Rudd's and Seltzer's cross sections is performed in an efficient manner.

2. Electron ionization cross sections

2.1. Rudd's model

The semi-empirical model of Rudd [Rudd 1990] is used for the electron ionization cross section. The differential cross section (DCS), written into two separate parts for convenience, is:

$$\frac{d\sigma_{ion}^i}{dw} = \frac{d\sigma_{ion}^{i(1)}}{dw} + \frac{d\sigma_{ion}^{i(2)}}{dw}, \quad (1)$$

where

$$\frac{d\sigma_{ion}^{i(1)}}{dw} = \frac{S_i}{I_i} F_1(t) \left[\frac{1}{(1+w)^3} + \frac{1}{(t-w)^3} - \frac{1}{(1+w)^{3/2}(t-w)^{3/2}} \right], \quad (2)$$

$$\frac{d\sigma_{ion}^{i(2)}}{dw} = \frac{S_i}{I_i} F_2(t) \left[\frac{1}{(1+w)^2} + \frac{1}{(t-w)^2} - \frac{1}{1+w} \frac{1}{t-w} \right]. \quad (3)$$

In equations (1-3), the dimensionless quantities $t = T/I_i$ and $w = W/I_i$ have been introduced, where T is the kinetic energy of the primary electron, W is the kinetic energy of the ejected electron and I_i is the binding energy of the electron in the i^{th} molecular orbital. The outer orbitals, by increasing ionization energies, are named 1b₁, 3a₁, 1b₂, 2a₁ and the inner orbital is 1a₁. Furthermore, $S_i = 4\pi a_0^2 N_i (\Re / I_i)^2$, a_0 is the Bohr radius (5.3×10^{-11} m), $\Re$ is the Rydberg energy (13.6 eV) and N_i is the number of electrons of the orbital. The functions F_1 and F_2 are given by

$$F_1(t) = A_1 \frac{\ln(t)}{t + B_1}, \quad (4)$$

$$F_2(t) = \frac{A_2}{t + B_2}. \quad (5)$$

The parameters A_1 , A_2 , B_1 and B_2 are given in Table 1.

Table 1. Parameters used in Rudd's equations.

i	Orbital	N _i	I _i (eV)	A ₁	A ₂	B ₁	B ₂
1	1b ₁	2	8.76	0.50	1.13	2.30	22.0
2	3a ₁	2	12.1	0.75	1.13	2.30	22.0
3	1b ₂	2	16.8	0.90	1.13	2.30	22.0
4	2a ₁	2	32.2	1.31	0.37	0.00	0.00
5	1a ₁	2	540	1.31	0.37	0.00	0.00

The total ionization cross section of the i^{th} molecular orbital is found by integration of the differential cross section

$$\sigma_{ion}^i = \int_0^{(T-I_i)/2} \frac{d\sigma_{ion}^i}{dW} dW. \quad (6)$$

The maximal possible energy of the secondary electron that can be observed is $(T-I_i)/2$ because the secondary electrons are indistinguishable from the scattered primaries. This integration gives

$$\sigma_{ion}^i = S_i F_1(t) \frac{t-1}{2t^2} \left(t + 1 - \frac{4\sqrt{t}}{3+t} \right) + S_i F_2(t) \left(1 - \frac{1}{t} - \frac{\ln(t)}{t+1} \right). \quad (7)$$

The Rudd's cross section yields excellent results for the calculation of range and stopping power below ~ 100 keV [Plante and Cucinotta 2009]. Above ~ 100 keV, if this formula is used without modifications, the cross section continues to drop as energy increases, and it is not possible to reproduce the plateau in the stopping power at high energies.

2.2. Seltzer's formula

Seltzer's cross section [Seltzer 1988] increases above ~ 1 MeV, which yields a relativistic rise in the stopping power that is observed in most elements [Gümüş 2005]. For the i^{th} orbital of a molecule, the differential cross-section in kinetic energy W of the ejected electron for an incident electron of kinetic energy T is written as the sum of two contributions: the close collision and the distant collision:

$$\frac{d\sigma_{ion}^i}{dW} = \frac{d\sigma_c^i}{dW} + \frac{d\sigma_d^i}{dW}. \quad (9)$$

The close collision term is given by

$$\frac{d\sigma_c^i}{dW} = \frac{2\pi r_e^2 m c^2 N_i}{\beta^2} \frac{T}{T + B_i + U_i} \left[\frac{1}{E^2} + \frac{1}{(T - W)^2} + \frac{1}{T^2} \left(\frac{\tau}{\tau + 1} \right)^2 - \frac{2\tau + 1}{(\tau + 1)^2} \frac{1}{E(T - W)} + G_i \right], \quad (10)$$

$$G_i = \frac{8U_i}{3\pi} \left[\frac{1}{E^3} + \frac{1}{(T - W)^3} \right] \left[\tan^{-1} \sqrt{y} + \frac{\sqrt{y}(y - 1)}{(y + 1)^2} \right], \quad (11)$$

where $r_e = 2.81794 \times 10^{-15}$ m is the “electron radius”, $\tau = T/mc^2$ is the kinetic energy in units of the electron rest mass, N_i is the number of electrons per orbital, B_i is the binding energy, U_i is the mean kinetic energy of the target electron in the orbital, $E = W + B_i$ is the energy transfer and $y = W/U_i$. The relativistic quantities β and γ are given by:

$$\beta^2 = \frac{v^2}{c^2} = 1 - \left(1 + \frac{T}{mc^2} \right)^{-2}, \quad (12)$$

$$\gamma = (1 - \beta^2)^{-1/2} = 1 + \frac{T}{mc^2}. \quad (13)$$

The distant collision part of the cross section can be written

$$\frac{d\sigma_d^i}{dW} = N_i I(E) \sigma_{PE}^i(E). \quad (14)$$

Here, $\sigma_{PE}^i(E)$ is the photoelectric cross section for the i^{th} molecular orbital of water for an incident photon of energy $E = W + B_i$. They are calculated from the atomic subshells photoelectric cross sections of hydrogen and oxygen by weighting each contribution by the parentage coefficients. These data are taken directly from [Uehara et al. 1992] and shown in Figure 1. The parameters of the molecular orbitals are given in Table 2.

The quantity $I(E)$ is the virtual-photon spectrum integrated over impact parameters $b_{\min} < b < b_{\max}$.

$$I(E) = \frac{2}{137\pi\beta^2 E} [G(x_{\min}) - H(x_{\max})], \quad (15)$$

where

$$G(x_{\min}) = x_{\min} K_0(x_{\min}) K_1(x_{\min}) - \frac{x_{\min}^2}{2} [K_1^2(x_{\min}) - K_0^2(x_{\min})], \quad (16)$$

$$H(x_{\max}) = x_{\max} K_0(x_{\max}) K_1(x_{\max}) - \frac{x_{\max}^2}{2} [K_1^2(x_{\max}) - K_0^2(x_{\max})]. \quad (17)$$

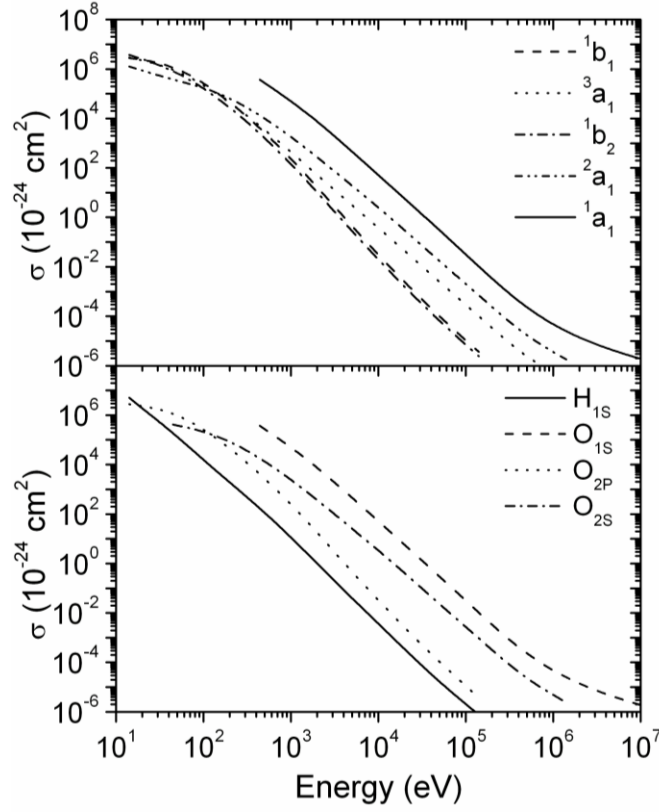


Figure 1: Photoelectric cross sections (top): orbitals of water molecule (bottom): atomic subshells H_{1s} , O_{1s} , O_{2s} and O_{2p} . These cross sections are used to calculate the contribution of the distant collision to the electron ionization cross section (see text).

Table 2. Parameters used in Seltzer's equation.

i	Orbital	N_i	B_i (eV)*	U_i (eV)	Parentage coefficients	$\langle r \rangle_i$
1	$1b_1$	2	11.50 (12.62)	30	1.000 O_{2p}	0.833
2	$3a_1$	2	11.75 (14.75)	40	0.175 H_{1s} 0.720 O_{2p} 0.105 O_{2s}	0.867
3	$1b_2$	2	14.3 (18.51)	50	0.410 H_{1s} 0.590 O_{2p}	0.901
4	$2a_1$	2	16.0 (32.4)	60	0.250 H_{1s} 0.750 O_{2s}	0.906
5	$1a_1$	2	539.7	700	1.000 O_{1s}	0.129

*The values given allow the cross sections to join smoothly at 50 keV, whereas the numbers in parenthesis are from [Uehara et al. 1992].

The quantities $x_{\min}$ and $x_{\max}$ are defined as

$$x_{\min} = \frac{Eb_{\min}}{\hbar c} \frac{\sqrt{1-\beta^2}}{\beta}, \quad (18)$$

$$x_{\max} = \frac{Eb_{\max}}{\hbar c} \frac{\sqrt{1-\beta^2}}{\beta}. \quad (19)$$

Here, $K_0(x)$ and $K_1(x)$ are the Modified Bessel Function of the Second Kind [Abramowitz and Stegun 1972] of order 0 and 1. The quantities $b_{\min}$ and $b_{\max}$ are impact parameters, where $b_{\min} = \langle r \rangle_i$ is the expected value of the electron radius for the orbital of interest and

$$b_{\max} = \frac{1.123\hbar c}{B_i} \frac{\beta}{\sqrt{1-\beta^2}}, \quad (20)$$

The ionization cross section for the i^{th} molecular orbital is given by:

$$\sigma_{ion}^i = \int_0^{(T-B_i)/2} \frac{d\sigma_{ion}^i}{dW} dW. \quad (21)$$

This integral must be evaluated numerically.

3. Sampling of the energy transfer

3.1. Sampling of the energy transfer from Rudd's cross section

We first note that the Rudd's total cross section is divided in two parts:

$$p_1 = S_i F_1(t) \frac{t-1}{2t^2} \left(t+1 - \frac{4\sqrt{t}}{3+t} \right), \quad (22)$$

$$p_2 = S_i F_2(t) \left(1 - \frac{1}{t} - \frac{\ln(t)}{t+1} \right). \quad (23)$$

As a first step, one can determine whether the sampling is performed using part 1 or part 2, using a probability proportional to their relative weight, $p_1/(p_1+p_2)$ and $p_2/(p_1+p_2)$.

If part 1 is sampled, we note that

$$\left[\frac{1}{(1+w)^3} + \frac{1}{(t-w)^3} - \frac{1}{(1+w)^{3/2}(t-w)^{3/2}} \right] \leq \left[\frac{1}{(1+w)^3} + \frac{1}{(t-w)^3} \right], \quad (24)$$

so, we can use a rejection method [Devroye, 1986]. The weights of the two parts are given by:

$$p_{1a} = \int_0^{(t-1)/2} \frac{1}{(1+w)^3} dw = \frac{1}{2} - \frac{2}{(1+t)^2}, \quad (25)$$

$$p_{1b} = \int_0^{(t-1)/2} \frac{1}{(t-w)^3} dw = -\frac{1}{2t^2} + \frac{2}{(1+t)^2}. \quad (26)$$

These functions can be sampled by inversion:

$$\int_0^{w_s} \frac{1}{(1+w)^3} dw = U \left(\frac{1}{2} - \frac{2}{(1+t)^2} \right), \quad (27)$$

$$\int_0^{w_s} \frac{1}{(t-w)^3} dw = U \left(-\frac{1}{2t^2} + \frac{2}{(1+t)^2} \right), \quad (28)$$

where U is a uniformly distributed random number between 0 and 1. After solving, we get

$$w_s = \frac{(t+1)}{\sqrt{(t+1)^2 - (t-1)(t+3)U}} - 1, \quad (29)$$

$$w_s = t - \frac{t(t+1)}{\sqrt{(t+1)^2 + (t-1)(3t+1)U}}, \quad (30)$$

where, again, U is a uniformly distributed random number between 0 and 1.

If part 2 is sampled, we proceed similarly. We note that

$$\left[\frac{1}{(1+w)^2} + \frac{1}{(t-w)^2} - \frac{1}{(1+w)(t-w)} \right] \leq \left[\frac{1}{(1+w)^2} + \frac{1}{(t-w)^2} \right], \quad (31)$$

so that we can use a rejection method as well. First calculate the weights of the two parts:

$$p_{2a} = \int_0^{(t-1)/2} \frac{1}{(1+w)^2} dw = \frac{t-1}{t+1}, \quad (32)$$

$$p_{2b} = \int_0^{(t-1)/2} \frac{1}{(t-w)^2} dw = \frac{t-1}{t(t+1)}. \quad (33)$$

The two remaining functions can be sampled by inversion as well,

$$\int_0^{w_s} \frac{1}{(1+w)^2} dw = U \left(\frac{t-1}{t+1} \right), \quad (34)$$

$$\int_0^{w_s} \frac{1}{(t-w)^2} dw = U \left(\frac{t-1}{t(t+1)} \right). \quad (35)$$

Solving for w_s yields

$$w_s = \frac{U(t-1)}{(t+1) - U(t-1)}, \quad (36)$$

$$w_s = \frac{t(t-1)U}{(t+1) + (t-1)U}. \quad (37)$$

3.2. Sampling of the energy transfer from Seltzer's cross section

Although $\frac{d\sigma_c^i}{dW}$ is very complex, it is a monotonically decreasing function of W , with the maximum at $W = 0$. Therefore,

$$\frac{d\sigma_c^i}{dW} \leq f_{\text{lim}}(W), \quad (38)$$

where

$$f_{\text{lim}}(W) = \begin{cases} \sigma_0 & , W < B_i \\ \sigma_0 \frac{2B_i^{3/2}}{W^2} & , W \geq B_i \end{cases}, \quad (39)$$

and $\sigma_0 = \frac{d\sigma_{\text{ion}}^i}{dW}(0)$ is used to simplify notation. It is possible to do a sampling algorithm by rejection using f_{lim} . First the weights are determined as

$$p_1 = \int_0^{B_i} \sigma_0 dW = \sigma_0 B_i, \quad (40)$$

$$p_2 = \int_{B_i}^{(t-B_i)/2} \frac{\sigma_0 2B_i^{3/2}}{W^2} dW = \sigma_0 2B_i^{3/2} \left(\frac{1}{B_i} + \frac{2}{t-B_i} \right). \quad (41)$$

The function can be sampled by inversion according to

$$\int_0^{W_s} \sigma_0 dW = U \sigma_0 B_i, \quad (42)$$

which leads to

$$W_s = B_i U, \quad (43)$$

where U is a uniform random number between 0 and 1. The sampling of the second part is done similarly

$$\int_{B_i}^{W_s} \frac{\sigma_0 2B_i^{3/2}}{W^2} dW = U \sigma_0 2B_i^{3/2} \left(\frac{1}{B_i} + \frac{2}{t-B_i} \right), \quad (44)$$

leading to

$$W_s = \frac{B_i(t-B_i)}{t-B_i + (3B_i - T)U}. \quad (45)$$

4. Verification and validation

4.1 The ionization cross sections by electrons

The ionization cross sections for electrons used in RITRACKS are shown in Figure 2. The cross sections join relatively smoothly, although a cutoff is seen at 50 keV.

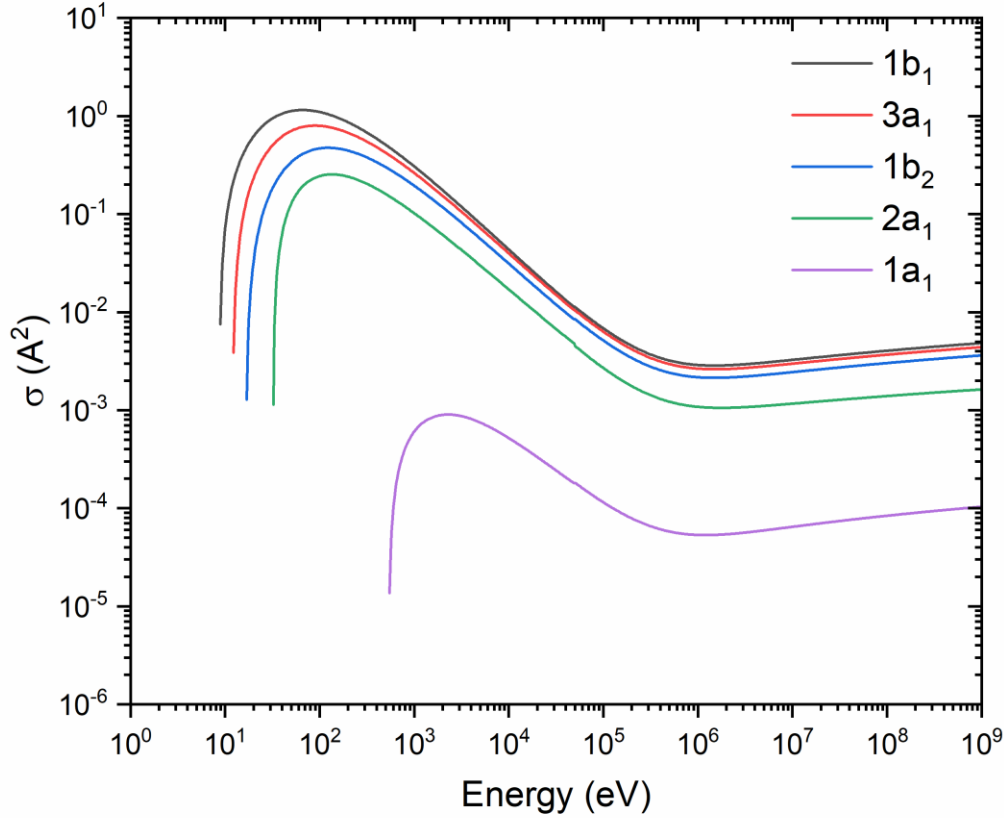


Figure 2. Electron ionization cross sections used in RITRACKS for the water molecular orbitals $1b_1$, $3a_1$, $1b_2$, $2a_1$ and $1a_1$. The Rudd's cross section is used for electron energies below 50 keV, and the Seltzer's cross section is used for those with energies higher than 50 keV.

4.2 Sampling of the ionization cross sections

The algorithms were verified and validated by using the algorithm 1,000,000 times (more at high energies) to generate energy loss values. These values were binned and normalized to the total cross section, and the results are compared with the differential cross section. This calculation was performed for electrons of various energies; an example of such calculation is shown in Figure 3 for the orbital $1b_1$ of water. The results are in excellent agreement with the analytical calculation for all initial electron energies. The difference between the sampling results (dots) and the analytical functions (lines) are barely noticeable, except at very high energies. This is due to the low probabilities associated with sampling high energies, which can be as high as 10 orders of magnitude lower.

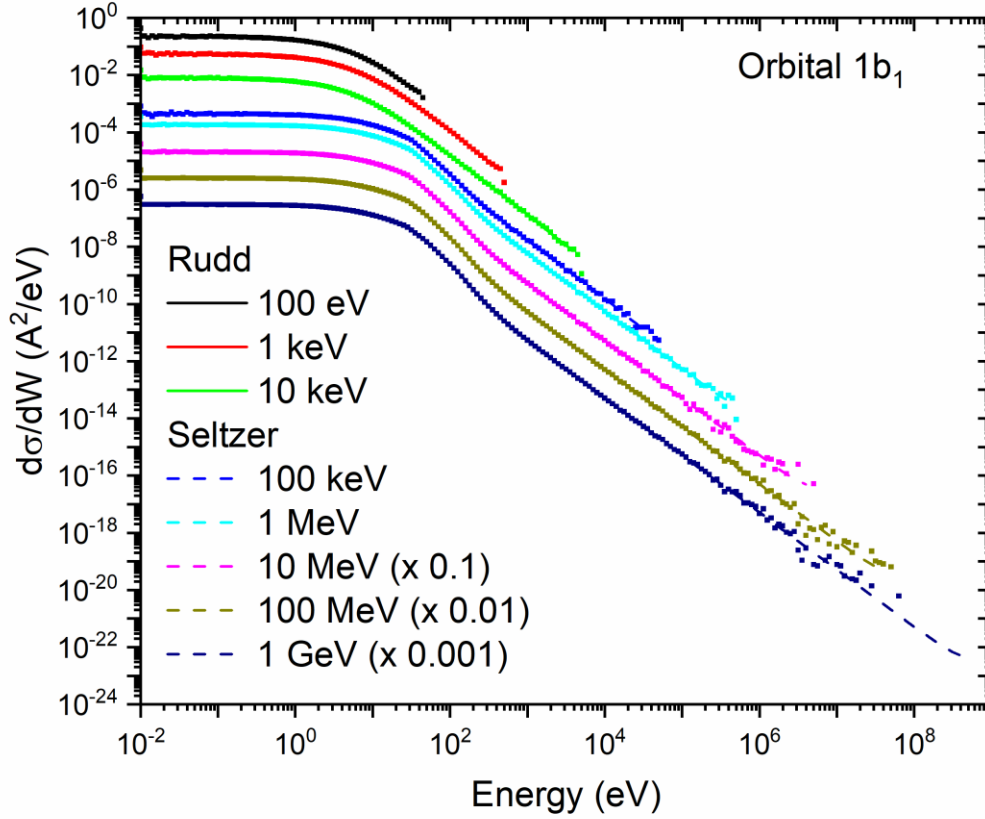


Figure 3: Sampling of the energy of the secondary electron for 10^2 , 10^3 , 10^4 , 10^5 and 10^6 eV incident electrons. Rudd's cross section is used below 5×10^4 eV and Seltzer's cross section is used above. The lines are the analytical predictions; the dots are the results of Monte-Carlo sampling.

5. Discussion

The electron cross sections are a fundamental quantity that are included in radiation transport codes. Most electrons generated during particle transport have energy below 50 keV, and many of them below 100 eV. During particle transport, these electrons ionize water molecules. It is therefore very important to have accurate and fast algorithms to perform the sampling of the energy loss at each interaction.

We note that the Rudd's and Seltzer's differential cross sections have similar shapes. The Rudd's cross section, however, is much simpler and easier to use. As most electrons generated during particle transport have energy below 50 keV, the algorithms described are very useful. Rudd's cross section is not sufficiently accurate to be used at high energies. Therefore, Seltzer's cross section is preferred at high energies. The Seltzer's algorithm is slower than Rudd's because it requires the calculation of Seltzer's cross section at each rejection step. However, only a small fraction of the electrons have energies higher than 50 keV, so the performance of the Seltzer's cross section sampling algorithm should have a negligible influence on the overall track structure simulation time.

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