G-value calculation program

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1 Compton effect

Following [1], we derive a differential cross section as a function of the electron energy T from the differential cross section per unit solid angle θ given by Klein and Nishina

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{r_0^2}{2} \frac{1}{(1 + \alpha(1 - \cos\theta))^2} \left(1 + \cos^2\theta + \frac{\alpha^2(1 - \cos\theta)^2}{(1 + \alpha(1 - \cos\theta))} \right),\tag{1}$$

where $r_0 = e^2/(mc^2)$, $\alpha = h\nu/(mc^2)$, e is the elementary charge, m is the electron mass, c is the speed of light and $h\nu$ is the energy of γ -ray. The solid angle is $d\Omega = \sin\theta d\theta d\varphi$. From the conservation laws, the electron energy T is written in terms of the photon deflection angle θ ,

$$T = h\nu \left(1 - \frac{1}{1 + \alpha(1 - \cos \theta)} \right). \tag{2}$$

Using the electron energy, we obtain

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{r_0^2}{2} \left(\frac{h\nu - T}{h\nu} \right)^2 \left[1 + \left(1 - \frac{T}{\alpha(h\nu - T)} \right)^2 + \frac{T^2}{(h\nu - T)h\nu} \right]. \tag{3}$$

By taking the derivative of T with respect to θ , we have

$$\frac{\mathrm{d}T}{\mathrm{d}\theta} = h\nu \frac{\alpha \sin \theta}{(1 + \alpha(1 - \cos \theta))^2}.$$
 (4)

Therefore, the differential cross section per unit energy T becomes

$$\frac{\mathrm{d}\sigma(T)}{\mathrm{d}T} = \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \left(2\pi \sin\theta \frac{\mathrm{d}\theta}{\mathrm{d}T} \right) = \frac{\pi r_0^2}{\alpha h \nu} \left[1 + \frac{T^2}{(h\nu - T)h\nu} + \left(1 - \frac{T}{\alpha(h\nu - T)} \right)^2 \right]. \tag{5}$$

Figure 1 shows the differential cross section per unit energy for three primary photon energies, $\alpha = 1, 2.35, 5.403$. The figure completely reproduces the result given in Fig. 49 of [1]. Figure 2 shows the differential cross section per unit energy for 60 Co γ -ray energy, $h\nu = 1.17, 1.33$ [MeV]. The graph looks similar to Fig. 1 of [4], but the vertical axis differs. But, I don't understand what f(T) is and its unit.

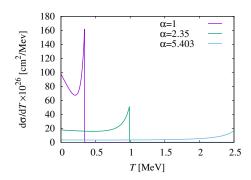


Figure 1: The differential cross section per unit energy for three primary photon energies, $\alpha = 1, 2.35, 5.403$.

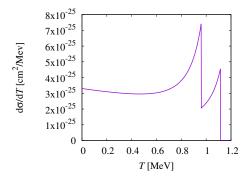


Figure 2: The differential cross section per unit energy for $^{60}{\rm Co}~\gamma$ -ray energy, $h\nu=1.17,1.33~{\rm [MeV]}.$

2 Cross section

The differential cross section 1 per unit of energy for the energy loss E of the incident electron with the energy T is given by

$$\sigma_E(T) = \sigma_{E,d} + \sigma_{E,e},\tag{6}$$

where the direct excitation and excitation induced by the exchange between the incident electron and an atomic electron are respectively given by

$$\sigma_{E,d}(T) = \frac{\pi e^4}{T + I_i + E_i} \left(\frac{1}{E^2} + \frac{4E_i}{3E^3} \right),\tag{7}$$

$$\sigma_{E,e}(T) = \frac{\pi e^4}{T + I_i + E_i} \left(\frac{1}{(T + I_i - E)^2} + \frac{4E_i}{3(T + I_i - E)^3} \right)$$
(8)

for $T + I_i - E \ge 0$. The subscript i = 1, 2, 3, ... signifies the shell (i = 1 is the outermost shell.) E_i and I_i are the average kinetic energy and the binding energy of the atomic electron under consideration. If the atomic electron is in the outermost shell of the atom, I_i is the ionization potential of the atom $I(I_1 = I)$.

3 Total cross section

3.1 Ionization

The total cross section for ionization is

$$Q_{\text{ion},i} = \frac{1}{2} \int_{I_i}^T \sigma_E dE = \int_{I_i}^{(T+I_i)/2} \sigma_E dE = \int_{I_i}^T \sigma_{E,d} dE.$$

$$(9)$$

The factor of 1/2 arises because we cannot distinguish whether the scattered electron is originally incidental or atomic. The second and third equalities are proven by using $E' = T + I_i - E$. We integrate σ_E over $E \in [I_i, (T + I_i)/2]$,

$$\int_{I_{i}}^{(T+I_{i})/2} \sigma_{E} dE = \frac{\pi e^{4}}{T + I_{i} + E_{i}} \int_{I_{i}}^{(T+I_{i})/2} \left(\frac{1}{E^{2}} + \frac{4E_{i}}{3E^{3}}\right) dE
+ \frac{\pi e^{4}}{T + I_{i} + E_{i}} \int_{I_{i}}^{(T+I_{i})/2} \left(\frac{1}{(T + I_{i} - E)^{2}} + \frac{4E_{i}}{3(T + I_{i} - E)^{3}}\right) dE
= \frac{\pi e^{4}}{T + I_{i} + E_{i}} \int_{I_{i}}^{(T+I_{i})/2} \left(\frac{1}{E^{2}} + \frac{4E_{i}}{3E^{3}}\right) dE
+ \frac{\pi e^{4}}{T + I_{i} + E_{i}} \int_{T}^{(T+I_{i})/2} \left(\frac{1}{E'^{2}} + \frac{4E_{i}}{E'^{3}}\right) (-dE')
= \int_{I_{i}}^{T} \sigma_{E,d} dE.$$
(10)

 $^{^{1}\}mathrm{The~unit~of~the~differential~cross~section~is~[charge]^{4}/[Energy]^{3}} = [\mathrm{dyn^{2}~cm^{4}/erg^{3}}] = [\mathrm{cm^{2}/erg}] = [\mathrm{s^{2}/g}].$

Similarly, we evaluate the integral of $\sigma_{E,e}$.

$$\int_{I_{i}}^{T} \sigma_{E,e} dE = \frac{\pi e^{4}}{T + I_{i} + E_{i}} \int_{I_{i}}^{T} \left(\frac{1}{(T + I_{i} - E)^{2}} + \frac{4E_{i}}{(T + I_{i} - E)^{3}} \right) dE$$

$$= \frac{\pi e^{4}}{T + I_{i} + E_{i}} \int_{T}^{I_{i}} \left(\frac{1}{E'} + \frac{4E_{i}}{E'^{3}} \right) (-dE')$$

$$= \int_{I_{i}}^{T} \sigma_{E,d} dE. \tag{11}$$

Therefore, (9) is proven. Now, we evaluate (9).

$$Q_{\text{ion},i} = \int_{I_i}^{T} \sigma_{E,d} dE = \frac{\pi e^4}{T + I_i + E_i} \int_{I_I}^{T} \left(\frac{1}{E^2} + \frac{4E_i}{3E^3} \right) dE$$

$$= \frac{\pi e^4}{T + I_i + E_i} \left[-\frac{1}{E} - \frac{2E_i}{3E^2} \right]_{I_i}^{T}$$

$$= \frac{\pi e^4}{T + I_i + E_i} \left[\left(\frac{1}{I_i} - \frac{1}{T} \right) + \frac{2E_i}{3} \left(\frac{1}{I_i^2} - \frac{1}{T^2} \right) \right]. \tag{12}$$

Figure 3 shows the total ionization cross section of hydrogen with $I_1 = 16.0[\text{eV}]$ and $E_1 = 31.96[\text{eV}]$. As in [3], the dissociative ionization and excitation are also considered. We are not able to reproduce the result of [3].

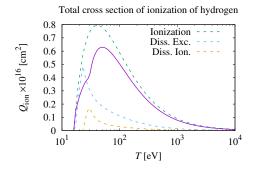


Figure 3: The total ionization cross section of hydrogen with $I_1 = 16.0$ [eV], $E_1 = 31.96$ [eV].

3.2 Singlet and Triplet

The cross section of excitations are given by

$$Q_{\operatorname{sngl},i} = Q_{\operatorname{de},i} + \frac{1}{2}Q_{\operatorname{ee},i},\tag{13}$$

$$Q_{\text{trpl},i} = \frac{1}{2} Q'_{\text{ee},i} \tag{14}$$

$$Q_{\mathrm{de},i}(T \ge I_i) = \int_{E_{s,i}}^{I_i} \sigma_{E,\mathrm{d}} \mathrm{d}E = \frac{\pi e^4}{T + I_i + E_i} \left[\left(\frac{1}{E_{s,i}} - \frac{1}{I_i} \right) + \frac{2E_i}{3} \left(\frac{1}{E_{s,i}^2} - \frac{1}{I_i^2} \right) \right],\tag{15}$$

$$Q_{\text{de},i}(E_{s,i} \le T < I_i) = \int_{E_{s,i}}^T \sigma_{E,\text{d}} dE = \frac{\pi e^4}{T + I_i + E_i} \left[\left(\frac{1}{E_{s,i}} - \frac{1}{T} \right) + \frac{2E_i}{3} \left(\frac{1}{E_{s,i}^2} - \frac{1}{T^2} \right) \right],\tag{16}$$

$$Q_{\mathrm{de},i}(T < E_{s,i}) = 0, \tag{17}$$

$$Q_{\text{ee},i}(T \ge I_i) = \int_{E_{s,i}}^{I_i} \sigma_{E,\text{e}} dE = \frac{\pi e^4}{T + I_i + E_i} \left[\left(\frac{1}{T} - \frac{1}{T + I_i - E_{s,i}} \right) + \frac{2E_i}{3} \left(\frac{1}{T^2} - \frac{1}{(T + I_i - E_{s,i})^2} \right) \right], \tag{18}$$

$$Q_{\mathrm{de},i}(E_{s,i} \le T < I_i) = \int_{E_{s,i}}^T \sigma_{E,e} dE = \frac{\pi e^4}{T + I_i + E_i} \left[\left(\frac{1}{I_i} - \frac{1}{T + I_i - E_{s,i}} \right) + \frac{2E_i}{3} \left(\frac{1}{I_i^2} - \frac{1}{(T + I_i - E_{s,i})^2} \right) \right], \tag{19}$$

$$Q_{ee,i}(T < E_{s,i}) = 0,$$
 (20)

$$Q'_{\text{ee}}(T \ge I_i) = \int_{E_{t,i}}^{I_i} \sigma_{E,\text{e}} dE = \frac{\pi e^4}{T + I_i + E_i} \left[\left(\frac{1}{T} - \frac{1}{T + I_i - E_{t,i}} \right) + \frac{2E_i}{3} \left(\frac{1}{T^2} - \frac{1}{(T + I_i - E_{t,i})^2} \right) \right], \tag{21}$$

$$Q'_{\text{ee},i}(E_{t,i} \le T < I_i) = \int_{E_{t,i}}^{T} \sigma_{E,\text{e}} dE = \frac{\pi e^4}{T + I_i + E_i} \left[\left(\frac{1}{I_i} - \frac{1}{T + I_i - E_{t,i}} \right) + \frac{2E_i}{3} \left(\frac{1}{I_i^2} - \frac{1}{(T + I_i - E_{t,i})^2} \right) \right], \tag{22}$$

$$Q'_{ee,i}(T < E_{t,i}) = 0, (23)$$

 $E_{s,i}$ and $E_{t,i}$ are the energies of the singlet and triplet levels of i-th shell, respectively.

4 Stopping power

The stopping power of the medium consists of a single kind of atom² is expressed as

$$S(T) = \sum_{i} S_i(T), \tag{24}$$

²The unit of the stopping power is [cross sec.][Energy]²/[Volume]=[cm/dyn erg²/cm³]=[dyn].

where

$$S_{i}(T \ge I_{i}) = Nn_{i} \left[\int_{I_{i}}^{(T+I_{i})/2} E\sigma_{E} dE + \int_{E_{s,i}}^{I_{i}} E\sigma_{E} dE + \frac{1}{2} \int_{E_{t,i}}^{E_{s,i}} E\sigma_{E,e} dE \right], \tag{25}$$

$$S_i(E_{s,i} \le T < I_i) = Nn_i \left[\int_{E_{s,i}}^T E\sigma_E dE + \frac{1}{2} \int_{E_{t,i}}^{E_{s,i}} E\sigma_{E,e} dE \right], \tag{26}$$

$$S_i(T < E_{s,i}) = Nn_i \frac{1}{2} \int_{E_{t,i}}^T E\sigma_{E,e} dE.$$
(27)

N is the number of atoms in a unit volume³, n_i the number of electrons in the *i*-th shell and $E_{s,i}$, $E_{t,i}$ are, respectively, the energies of the lowest singlet and triplet levels of the *i*-th shell. We analytically evaluate the integral. The indefinite integrals to be evaluated are

$$\int \frac{E}{(T+I_{i}-E)^{2}} dE = \int \frac{-(T+I_{i}-E)+(T+I_{i})}{(T+I_{i}-E)^{2}} dE
= -\int \frac{1}{T+I_{i}-E} dE + (T+I_{i}) \int \frac{1}{(T+I_{i}-E)^{2}} dE
= \ln(T+I_{i}-E) + \frac{T+I_{i}}{T+I_{i}-E}.$$
(28)
$$\int \frac{E}{(T+I_{i}-E)^{3}} dE = \int \frac{-(T+I_{i}-E)+(T+I_{i})}{(T+I_{i}-E)^{3}} dE
= -\int \frac{1}{(T+I_{i}-E)^{2}} dE + (T+I_{i}) \int \frac{1}{(T+I_{i}-E)^{3}} dE
= -\frac{1}{T+I_{i}-E} + \frac{T+I_{i}}{2(T+I_{i}-E)^{2}},$$
(29)

$$\int \frac{E}{E^2} dE = \ln E, \tag{30}$$

$$\int \frac{E}{E^3} dE = -\frac{1}{E}.$$
(31)

³At the standard temperature and pressure (0°C and 1atm=101.325kPa; the former IUPAP definition until 1982), the molar volume of a gas is 22.4 litre. Then, $N = 6.02 \times 10^{23}/(22.4 \times 10^3) = 0.269 \times 10^{20}$ [cm⁻³]. For a solid, $N = d/(M/N_A)$ with d, M, $N_A \equiv 6.02 \times 10^{23}$ being the density, molecular weight and Avogadro number, respectively.

For $T < E_{s,i}$, we obtain

$$S_{i}(T < E_{s,i}) = N \frac{n_{i}}{2} \int_{E_{t,i}}^{T} E \sigma_{E,e} dE$$

$$= N \frac{n_{i}}{2} \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\ln(T + I_{i} - E) + \frac{T + I_{i}}{T + I_{i} - E} \right]$$

$$+ \frac{4E_{i}}{3} \left(-\frac{1}{T + I_{i} - E} + \frac{T + I_{i}}{2(T + I_{i} - E)^{2}} \right) \Big|_{E_{t,i}}^{T}$$

$$= N n_{i} \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\frac{1}{2} \ln \frac{I_{i}}{T + I_{i} - E_{t,i}} + \frac{1}{2} \frac{T + I_{i}}{I_{i}} - \frac{1}{2} \frac{T + I_{i}}{T + I_{i} - E_{t,i}} + \frac{2E_{i}}{3} \left(-\frac{1}{I_{i}} + \frac{1}{T + I_{i} - E_{t,i}} + \frac{T + I_{i}}{2I_{i}^{2}} - \frac{T + I_{i}}{2(T + I_{i} - E_{t,i})^{2}} \right) \right]. \tag{33}$$

For $E_{s,i} \leq T < I_i$, we obtain

$$\begin{split} S_{i}(E_{s,i} \leq T < I_{i}) &= Nn_{i} \int_{E_{s,i}}^{T} E\sigma_{E} \mathrm{d}E + N\frac{n_{i}}{2} \int_{E_{t,i}}^{E_{s,i}} E\sigma_{E,e} \mathrm{d}E \\ &= Nn_{i} \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\ln E - \frac{4E_{i}}{3E} \right]_{E_{s,i}}^{T} \\ &+ Nn_{i} \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\ln (T + I_{i} - E) + \frac{T + I_{i}}{T + I_{i} - E} \right. \\ &+ \frac{4E_{i}}{3} \left(-\frac{1}{T + I_{i} - E} + \frac{T + I_{i}}{2(T + I_{i} - E)^{2}} \right) \right]_{E_{s,i}}^{T} \\ &+ N\frac{n_{i}}{2} \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\ln (T + I_{i} - E) + \frac{T + I_{i}}{T + I_{i} - E} \right. \\ &+ \frac{4E_{i}}{3} \left(-\frac{1}{T + I_{i} - E} + \frac{T + I_{i}}{2(T + I_{i} - E)^{2}} \right) \right]_{E_{t,i}}^{E_{s,i}} \\ &= Nn_{i} \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\ln \frac{T}{E_{s,i}} + \ln \frac{I_{i}}{T + I_{i} - E_{s,i}} + \frac{1}{2} \ln \frac{T + I_{i} - E_{s,i}}{T + I_{i} - E_{t,i}} \right. \\ &- \frac{4E_{i}}{3} \left(\frac{1}{T} - \frac{1}{E_{s,i}} \right) + \frac{T + I_{i}}{I_{i}} - \frac{T + I_{i}}{T + I_{i} - E_{s,i}} \\ &+ \frac{4E_{i}}{3} \left(-\frac{1}{I_{i}} + \frac{1}{T + I_{i} - E_{s,i}} + \frac{T + I_{i}}{2I_{i}^{2}} - \frac{T + I_{i}}{2(T + I_{i} - E_{s,i})^{2}} \right) \\ &+ \frac{1}{2} \frac{T + I_{i}}{T + I_{i} - E_{s,i}} - \frac{1}{2} \frac{T + I_{i}}{T + I_{i} - E_{t,i}} \\ &+ \frac{2E_{i}}{3} \left(-\frac{1}{T + I_{i} - E_{s,i}} + \frac{1}{T + I_{i} - E_{t,i}} + \frac{T + I_{i}}{2(T + I_{i} - E_{s,i})^{2}} - \frac{T + I_{i}}{2(T + I_{i} - E_{s,i})^{2}} \right. \\ &+ 1 + \frac{T}{I_{i}} - \frac{T + I_{i}}{2(T + I_{i} - E_{s,i})} - \frac{T^{2}I_{i}^{2}}{2(T + I_{i} - E_{s,i})} \left. - \frac{T + I_{i}}{2(T + I_{i} - E_{t,i})} \right. \\ &+ \frac{E_{i}}{3} \left(-\frac{4}{T} + \frac{4}{E_{s,i}} - \frac{4}{I_{i}} + \frac{2}{T + I_{i} - E_{s,i}} + \frac{2}{T + I_{i} - E_{t,i}} \right) \\ &+ \frac{E_{i}}{3} \left(-\frac{4}{T} + \frac{4}{E_{s,i}} - \frac{4}{I_{i}} + \frac{2}{T + I_{i} - E_{s,i}} + \frac{2}{T + I_{i} - E_{t,i}} \right) \right]. \end{split}$$

For $T > I_i$, we first evaluate the singlet and triplet excitations using the previous result.

$$\int_{E_{s,i}}^{I} E \sigma_{E} dE + \frac{1}{2} \int_{E_{t,i}}^{E_{s,i}} E \sigma_{E,e} dE = \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\ln \frac{I_{i}}{E_{s,i}} + \ln \frac{T}{T + I_{i} - E_{s,i}} + \frac{1}{2} \ln \frac{T + I_{i} - E_{s,i}}{T + I_{i} - E_{t,i}} \right. \\
\left. - \frac{4E_{i}}{3} \left(\frac{1}{I_{i}} - \frac{1}{E_{s,i}} \right) + \frac{T + I_{i}}{T} - \frac{T + I_{i}}{T + I_{i} - E_{s,i}} \right. \\
\left. + \frac{4E_{i}}{3} \left(- \frac{1}{T} + \frac{1}{T + I_{i} - E_{s,i}} + \frac{T + I_{i}}{2T^{2}} - \frac{T + I_{i}}{2(T + I_{i} - E_{s,i})^{2}} \right) \right. \\
\left. + \frac{1}{2} \frac{T + I_{i}}{T + I_{i} - E_{s,i}} - \frac{1}{2} \frac{T + I_{i}}{T + I_{i} - E_{t,i}} \right. \\
\left. + \frac{2E_{i}}{3} \left(- \frac{1}{T + I_{i} - E_{s,i}} + \frac{1}{T + I_{i} - E_{t,i}} + \frac{T + I_{i}}{2(T + I_{i} - E_{s,i})^{2}} - \frac{T + I_{i}}{2(T + I_{i} - E_{t,i})^{2}} \right) \right] \\
= \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\frac{1}{2} \ln \frac{I_{i}^{2}T^{2}}{E_{s,i}^{2}(T + I_{i} - E_{s,i})(T + I_{i} - E_{t,i})} + \frac{I_{i}}{2(T + I_{i} - E_{t,i})} + \frac{I_{i}}{2(T + I_{i} - E_{s,i})} - \frac{T + I_{i}}{2(T + I_{i} - E_{t,i})} + \frac{E_{i}}{3} \left(- \frac{4}{I_{i}} + \frac{4}{E_{s,i}} - \frac{4}{T} + \frac{2}{T + I_{i} - E_{s,i}} + \frac{2}{T + I_{i} - E_{t,i}} \right) \\
\left. + \frac{E_{i}}{3} \left(T + I_{i} \right) \left(\frac{2}{T^{2}} - \frac{1}{(T + I_{i} - E_{s,i})^{2}} - \frac{1}{(T + I_{i} - E_{t,i})^{2}} \right) \right]. \tag{35}$$

The first term becomes

$$\int_{I_{i}}^{\frac{(T+I_{i})}{2}} E\sigma_{E} dE = \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\ln E - \frac{4E_{i}}{3E} \right]_{I_{i}}^{(T+I_{i})/2}
+ \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\ln (T + I_{i} - E) + \frac{T + I_{i}}{T + I_{i} - E} \right]
+ \frac{4E_{i}}{3} \left(-\frac{1}{T + I_{i} - E} + \frac{T + I_{i}}{2(T + I_{i} - E)^{2}} \right)_{I_{i}}^{(T+I_{i})/2}
= \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\ln \frac{T + I_{i}}{2I_{i}} + \ln \frac{T + I_{i}}{2T} - \frac{4E_{i}}{3} \left(\frac{2}{T + I_{i}} - \frac{1}{I_{i}} \right) \right]
+ 2 - \frac{T + I_{i}}{T} + \frac{4E_{i}}{3} \left(-\frac{2}{T + I_{i}} + \frac{1}{T} + \frac{2}{T + I_{i}} - \frac{T + I_{i}}{2T^{2}} \right)$$

$$= \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\ln \frac{(T + I_{i})^{2}}{4TI_{i}} + 1 - \frac{I_{i}}{T} + \frac{4E_{i}}{3} \left(\frac{1}{I_{i}} + \frac{1}{2T} - \frac{2}{T + I_{i}} - \frac{I_{i}}{2T^{2}} \right) \right]. \tag{36}$$

Combining the terms, we finally obtain

$$S_{i}(T \geq I_{i}) = Nn_{i} \frac{\pi e^{4}}{T + I_{i} + E_{i}} \left[\frac{1}{2} \ln \frac{(T + I_{i})^{4}}{16E_{s,i}^{2}(T + I_{i} - E_{s,i})(T + I_{i} - E_{t,i})} + 2 - \frac{T + I_{i}}{2(T + I_{i} - E_{s,i})} - \frac{T + I_{i}}{2(T + I_{i} - E_{t,i})} + \frac{1}{T + I_{i} - E_{t,i}} + \frac{1}{T + I_{i} - E_{t,i}} - \frac{T + I_{i}}{2(T + I_{i} - E_{s,i})^{2}} - \frac{T + I_{i}}{2(T + I_{i} - E_{t,i})^{2}} \right].$$

$$(37)$$

5 Degradation spectrum

The degradation spectrum of the incident electron is expressed as

$$y_1(T) = \frac{1}{S(T)}.$$
 (38)

To describe the degradation spectrum of secondary electrons, we modify the differential cross section of ionization by replacing T by T_1 and E by $T_2 + I_i$,

$$\sigma(T_1, T_2) = \frac{\pi e^4}{T_1 + I_i + E_i} \left[\frac{1}{(T_2 + I_i)^2} + \frac{4E_i}{3(T_2 + I_i)^3} + \frac{1}{(T_1 - T_2)^2} + \frac{4E_i}{3(T_1 - T_2)^2} \right],\tag{39}$$

for $T_1 \ge T_2$, where T_1 is the energy of incident electron, T_2 is the energy of secondary electron.y The degradation spectrum of the secondary electrons is

$$y_2(T) = \frac{N}{S(T)} \sum_{i} n_i \int_{T}^{(T_{\rm in} - I_i)/2} \int_{2T_2 + I_i}^{T_{\rm in}} y_1(T_1) \sigma(T_1, T_2) dT_1 dT_2.$$
 (40)

The integration range is shown in Fig. 4. The generated energy by collisions T_2 cannot exceed $(T_{\rm in} - I_i)/2$ with $T_{\rm in}$ being the incident electron energy by definition. The incident electron energy for the secondary is $T_{\rm in}$, that for the tertiary is the maximum energy of the secondary $(T_{\rm in} - I_i)/2$, and so on. The energy of incident electron T_1 must be greater than $2T_2 + I_i$ because the energy of the incident electron after the collision (T_1') must be greater than T_2 while the relation $T_1 = T_1' + T_2 + I_i$ must hold. Similar to the secondary, the degradation spectrum for the tertiary electrons is given by

$$y_3(T) = \frac{N}{S(T)} \sum_{i} n_i \int_{T}^{(T_{\rm in} - 3I_i)/4} \int_{2T_2 + I_i}^{(T_{\rm in} - I_i)/2} y_2(T_1) \sigma(T_1, T_2) dT_1 dT_2.$$
 (41)

And, similar equations can be constructed for the electrons in the later steps. The total degradation spectrum is the sum of the above:

$$y(T) = \sum_{m} y_m(T). \tag{42}$$

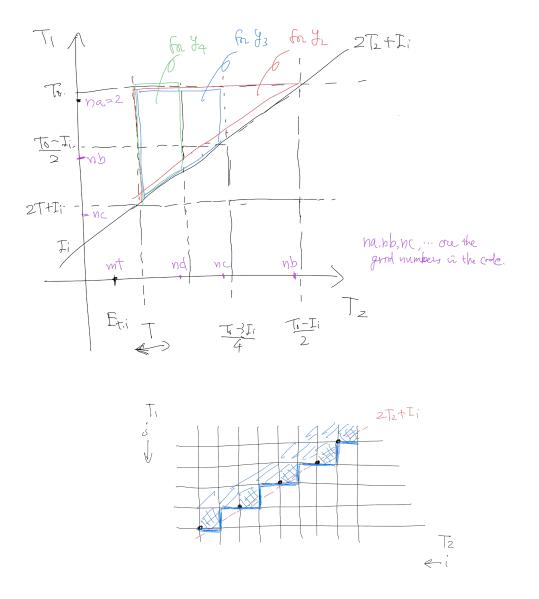


Figure 4: The integration range. The bottom figure shows the enlarged area along the $T_1=2T_2+I_i$ line.

5.1 Numerical evaluation

The energy grid is given by

$$\ln T_i = \ln T_{\rm in} + i \ln \Delta T \tag{43}$$

where ΔT is chosen to be $(1/2)^{1/N_{\rm div}} < 1$ with $N_{\rm div}$ being an input parameter. Inversely, for a given energy T, the mesh point given by

$$i = \left\lceil \frac{\ln \frac{T}{T_{\text{in}}}}{\ln \Delta T} + 1 \right\rceil \tag{44}$$

means the smallest energy grid greater than T (i.e., $T_{i+1} < T \le T_i$). The mesh point of T_{in} is i = 1. The integral is simply evaluated by

$$\int_{T}^{(T_{\rm in}-I_i)/2} \int_{2T_2+I_i}^{T_{\rm in}} y_1(T_1)\sigma(T_1, T_2) dT_1 dT_2 \approx \sum_{i} \sum_{j} y_1(T_j)\sigma(T_j, T_i)(T_{i-1} - T_i)(T_{j-1} - T_j).$$
 (45)

5.2 Results

We calculate the degradation spectrum for Helium. The parameters for Helium [5] are $E_{s,1} = 21.2$, $E_{t,1} = 19.8$, $I_1 = 24.581$, $E_1 = 38.74$ [eV], $n_1 = 2$ is used. The incident electron energy is $T_{\rm in} = 10^5$ [eV]. The result is shown in Fig. 5, fully reproducing Fig. 1 of [5].

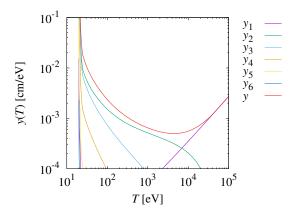


Figure 5: The degradation spectrum in Helium.

Figure 6 shows the degradation spectrum in water (gas phase) with the incident electron energy $T_{\rm in} = 10^5 [{\rm eV}]$. The figure looks different from Fig. 5 of [4] probably because the electron distribution generated by 60 Co γ -ray is not taken into account here.

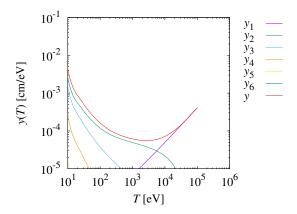


Figure 6: The degradation spectrum in water (gas phase).

Table 1: The parameters used for water [4].

Shell (i)	I_i	E_i	$E_{s,i}$	$E_{t,i}$	n_i
1	12.6	70.40	7.42	5.0	2
2	14.7	66.46	9.50	7.0	2
3	18.4	28.41	13.0	11.0	2
4	32.2	74.94	27.0	25.0	2
5	539.7	799.60	535.0	533.0	2

6 G value

Once the degradation spectrum y(T) is obtained, the calculation of the yields of excitation and ionization per incident electron is straightforward. The number of the species produced in the process s is given by

$$N_{s} = N \sum_{i} n_{i} \int_{T_{s}}^{T_{\text{in}}} y Q_{s,i} dT = N \sum_{i} n_{i} \int_{T_{s}}^{T_{\text{in}}} T y Q_{s,i} d \ln T,$$
(46)

where T_s is the threshold energy of the incident electron for the s process. The radiation yield (the G value) is the number of molecules formed per 100[eV] defined as

$$G_s = \frac{100N_s}{T_{\rm in}}.\tag{47}$$

Figure 7 is the TyQ plot showing the contribution of the electron slowing-down spectrum to the ionization and excitations. The G values are 2.53 (ionization), 4.10 (singlet) and 0.787 (triplet).

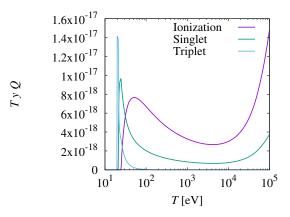


Figure 7: The TyQ plot for Helium.

7 Range and mean free path

The mean free path is defined by

$$\lambda = \frac{1}{N \sum_{s} Q_s} \tag{48}$$

The stopping power is the rate by which the electron loose the energy per unit length, S = dT/dx. Then, the length that electron can travel (the range) is given by [6]

$$R = \int_0^R \mathrm{d}x = \int_{T_{\rm in}}^0 \frac{\mathrm{d}T}{\mathrm{d}T/\mathrm{d}x} \sim \int_{T_{\rm in}}^{\min(E_{t,i})} \frac{T}{S} \mathrm{d}\ln T. \tag{49}$$

(Note that S is singular at $T = E_t$ and the integral does not converge. This definition must be re-considered.) Figure 8 shows the mean free path and range for helium with the incident electron energy $T_{\rm in} = 10^5 [{\rm eV}]$.

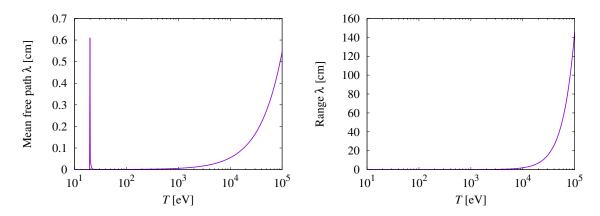


Figure 8: The mean free path and range for Helium.

A Constants and units

Basic physical constants are given in Table 2. Table 3 summarizes the derived quantities. The classical electron radius is given by $r_0 = e^2/(mc^2)$ with e given in the cgs-electrostatic unit, while $r_0 = e^2/(4\pi\epsilon_0 mc^2)$ with e in the SI unit. The conversion of C to statC is given by 1[C] = 10c[statC].

Table 2: Numerical values of basic constants. Adapted from [2].

Symbol	Name	Value	Unit [esu]	Value	Unit [SI]
\overline{e}	elementary charge	4.8032×10^{-10}	statC	1.6022×10^{-19}	$C=A\cdot s$
m	electron masse	9.1094×10^{-28}	g	9.1094×10^{-31}	$_{ m kg}$
c	speed of light	2.9979×10^{10}	${ m cm~s^{-1}}$	2.9979×10^{8}	${ m m~s^{-1}}$

Table 3: Derived quantities.

Symbol	Name	Value	
mc^2	electron rest mass energy	$0.510999 \; [MeV]$	$8.18711 \times 10^{-14} [J]$
r_0	classical electron radius	$2.8179 \times 10^{-13} \text{ [cm]}$	$2.8179 \times 10^{-15} \text{ [m]}$

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