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A Monte Carlo Study of Low-Energy Electron Transport in Liquid Water: Influence of the Rutherford Formula and the Mott Model *

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Influence of the Rutherford formula and the Mott model on the Monte Carlo simulation of low-energy electron (< 10 keV) transport in liquid water is investigated. One of the features of the constructed Monte Carlo code is the implementation of the new optical-data model from Emfietzoglou et al. in inelastic cross section based on the dielectric response theory. In addition, a novel mean elastic cross section by means of the Mott model is proposed to calculate the electron elastic scattering for high simulation efficiency. The systematical calculations of both the distribution of energy depositions and penetration parameter for low-energy electrons in liquid water are performed by using the Rutherford formula and the Mott model, respectively, for the elastic collisions in the simulations. The calculated results show that the effect of the two models is evident at energies below about 1 keV.

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Monte Carlo simulation of the track structure of charged particle in biological materials is very important for mechanistic studies of radiation effects in many fields, such as radiation biology, radiotherapy, space radiation and microdosimetry. The simulation of electron track structure in water is a fundamental work in studies of radiation biological effects.[1]

In Monte Carlo calculations of the track structures of low-energy electrons in liquid water, elastic and inelastic interactions of electrons with water represent scattering events that need to be exactly modeled. Based on the dielectric response theory, great effort[2−9] has been made for providing the cross sections of describing inelastic interactions between low-energy electrons (< 10 keV) and liquid water. A central problem in these works is the evaluation of the energy loss function (ELF), whereas the low-energy Born-correction for electron inelastic cross sections from the dielectric model is also a subject of long-standing theoretical interest because of the use of the first Born approximation in this model. To this end, detailed studies[4−12] have been carried out for examining the reliability of the evaluation of the ELF and for exploring the effectiveness of the different low-energy Born-corrections. For the simulation of the elastic scattering of low-energy electron in liquid water, the commonly used model is the Rutherford formula with the screening parameter,[1] moreover, the Mott model is applied in a few works.[5,9,13] However, the studies of the influence of different elastic scattering models on the track structure simulations of low-energy electrons in liquid water are sparse.

In this Letter, we investigate the influence of the two fundamental elastic scattering models, i.e. the Rutherford formula and the Mott model, on the simulation of low-energy electron (< 10 keV) transport in liquid water. The inelastic cross sections for energetic electrons in liquid water are derived from the dielectric response theory, based on the implementation of the optical-data model newly developed by Emfietzoglou *et al.*[12] Using the models presented in this work, we systematically calculate the spatial distributions of energy depositions of low-energy electrons in liquid water, and also simulate the penetration parameters of low-energy electrons in liquid water.

The Rutherford differential cross section with the screening parameter[1] is expressed by

$$\frac{d\sigma}{d\Omega} = \frac{Z(Z+1)r_e^2[(1-\beta^2)/\beta^4]}{(1-\cos\theta+2\eta)^2}, \tag{1}$$

where $Z = 7.42$ is the effect atomic number of water molecule, $r_e = 2.8179 \times 10^{-13}$ cm, β is given by

$$\beta^2 = 1 - \frac{1}{(T/m_0c^2+1)^2}, \tag{2}$$

and the screening parameter η is calculated by using

$$\eta = \eta_c \frac{1.7 \times 10^{-5} Z^{2/3} m_0c^2}{T(T/m_0c^2+2)}. \tag{3}$$

In Eqs. (2) and (3), T is the kinetic energy of the incident electron, $m_0c^2 = 511003.4$ eV is the electron rest mass energy, and $\eta_c = 1.198$ for $T < 50$ keV. From Eq. (1), the angular distribution of electron elastic scattering is obtained by

$$\cos\theta = 1 - \frac{2\eta R}{1+\eta-R}, \tag{4}$$

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where R is the random number distributed uniformly between zero to 1.

The Mott differential cross section derived from the relativistic wave equation of Dirac can be written as

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2, \tag{5}$$

where θ is the elastic scattering angle, and $f(\theta)$ and $g(\theta)$ are the scattering amplitudes.

The $f(\theta)$ and $g(\theta)$ can be expressed by partial wave expansions,[14] i.e.

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}\{(l+1)[\exp(2i\delta_l)-1] + l[\exp(2i\delta_{-l-1})-1]\}p_l(\cos\theta), \tag{6}$$

$$g(\theta) = \frac{1}{2ik}\sum_{l=1}^{\infty}[\exp(2i\delta_{-l-1}) - \exp(2i\delta_l)]p_l^1(\cos\theta), \tag{7}$$

where $p_l(\cos\theta)$ and $p_l^1(\cos\theta)$ are the ordinary and associated Legendre polynomials, respectively, and δ_l is the phase shift corresponding to lth partial wave, for which the detailed calculation principles can be found elsewhere.[14] Very recently, employing the partial wave method, Muñoz *et al.*[15] and Ma *et al.*[16,17] have calculated the cross sections of electron elastic scattering in complex polyatomic molecules including water molecule at low energies.

On the basis of the idea of mean cross section,[18] we propose the following method for the calculation of the elastic scattering of energetic electron in liquid water for high simulation efficiency.

For an electron with energy T, the mean differential cross section for each atom is given by

$$\frac{d\bar{\sigma}}{d\Omega} = \frac{n_{\rm H}}{n}\frac{d\sigma_{\rm H}}{d\Omega} + \frac{n_{\rm O}}{n}\frac{d\sigma_{\rm O}}{d\Omega}, \tag{8}$$

where the subscript corresponds to H or O in H_2O, $n_{\rm H}$ and $n_{\rm O}$ denote the atomic density of H and O, respectively, and $n = n_{\rm H} + n_{\rm O}$.

The total mean elastic cross section for each atom can be calculated from

$$\bar{\sigma} = \int_0^{\pi} 2\pi\left(\frac{d\bar{\sigma}}{d\Omega}\right)\sin\theta d\theta. \tag{9}$$

The elastic scattering angle can be obtained by

$$R = \int_0^{\theta}\left(\frac{d\bar{\sigma}}{d\Omega}\right)\sin\theta d\theta \Big/ \int_0^{\pi}\left(\frac{d\bar{\sigma}}{d\Omega}\right)\sin\theta d\theta, \tag{10}$$

where R is the random number as that in Eq. (4). It is clear that using the mean cross section the simulation of the elastic scattering is obviously simplified.

Figure 1 displays the total elastic cross sections calculated based on the Mott model and on the database of the National Institute of Standards and Technology (NIST)[14] for a H_2O molecule. The experiments from Katase *et al.*[19] and Danjo and Nishimura (DN),[20] the Rutherford cross sections,[1] and theoretical calculations of Muñoz *et al.*[15] are also plotted in this figure for comparison. It can be seen that the cross sections by the Mott model are in good agreement with those from Katase *et al.*, Danjo and Nishimura, and Muñoz *et al.*. However, it is also clear that the Rutherford cross-sections are different obviously from the others. Taking notice of the facts that the Rutherford cross section is obtained on the basis of classical mechanics principle and the Mott cross section is derived from a more exact treatment of elastic scattering, i.e. from quantum mechanics method, the difference between both the cross sections results from the two different theoretical methods used for deriving the electron elastic cross section.

A fitting to the total elastic cross sections from NIST data has been made for the convenient calculation in Monte Carlo simulation and for the extension to the lower energy, and the resultant fitting becomes

$$\sigma_e = \exp(-33.1827 - 0.3975u - 0.03035u^2), \tag{11}$$

where σ_e is the total elastic cross section in $\rm cm^2$ for a H_2O molecule and $u = \ln T$. This fitting is also presented in Fig. 1 for comparison. In the present work we use Eq. (11) to calculate σ_e in the energy range from a few eV to 10 keV.

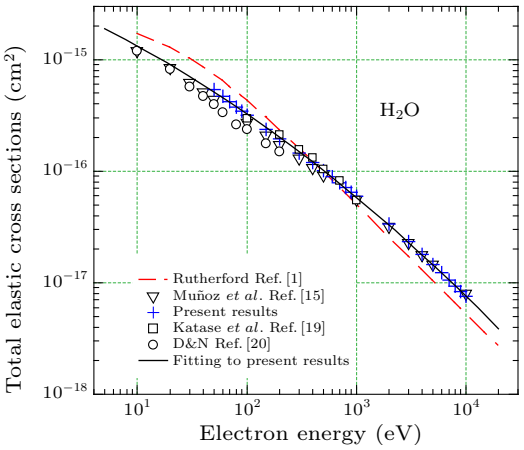

Fig. 1. Total elastic cross section as a function of incident electron energy. The present results are obtained based on the Mott model and on the database of the National Institute of Standards and Technology (NIST).[14]

In Fig. 2, the probability distributions for elastic scattering angle obtained from Eq. (10) at energies 200, 500 and 1000 eV are compared with those from the experiments[19,20] as well as the Rutherford formula.[1] At 200 eV the difference between the theoretical calculations and the experiments is evident, and at 500 and 1000 eV the results due to Eq. (10) are closer to the experiments than those by the Rutherford formula. According to this, we have constructed the probability tables of sampling elastic scattering

angle by using the data of Danjo and Nishimura[20] at energies of $T < 100\,\text{eV}$, the data of Katase *et al.*[19] in the range from 100 to 500 eV, and the differential cross section values due to Eq. (8) that is based on the Mott model for $T > 500\,\text{eV}$.

Following the dielectric response theory and taking into account the exchange correction based on the Ochkur approximation,[21] the differential cross section for low-energy electron inelastic scattering can be expressed as

$$\frac{d\sigma_{\text{in}}}{dE} = \frac{1}{\pi N a_0 T}\int_{q_-}^{q_+}\frac{1}{q}\text{Im}[-1/\varepsilon(q,E)]C_{\text{ex}}dq, \quad (12)$$

where σ_{in} is the microscopic inelastic cross section in units of area per target molecule, E and q are the energy loss and the momentum transfer, respectively, from the incident electron into a medium described by the complex dielectric response function $\varepsilon(q,E)$, $q_\pm = \sqrt{2m}(\sqrt{T} \pm \sqrt{T-E})$ with m the mass of electron, a_0 is the Bohr radius, N is the density of target, and

$$C_{\text{ex}} = 1 - \frac{q^2/2m}{T} + \left(\frac{q^2/2m}{T}\right)^2. \quad (13)$$

According to Emfietzoglou and Nikjoo,[11] we employ the classical Coulomb-field correction[22] in this work for the first Born approximation. This correction can be made by an increase of the incident electron's kinetic energy, i.e. by replacing T with $T + 2E_j$ for the excitation and by changing T to $T+B_j+U_j$ for the ionization, where E_j is the excitation energy for the jth discrete transition, B_j and U_j are the electron binding and kinetic energy in the jth shell, respectively, and the values of B_j and U_j were given in Ref. [23].

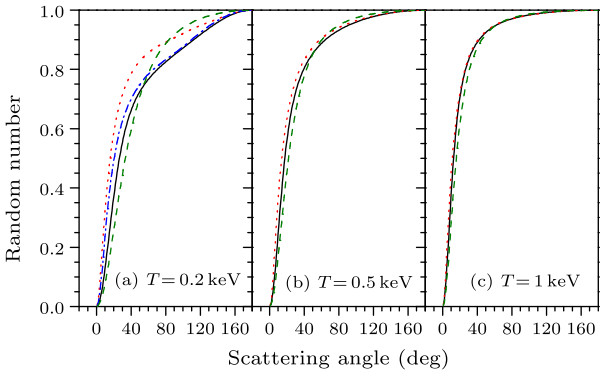

Fig. 2. Probability distributions for elastic scattering angle at energies: (a) $T = 0.2\,\text{keV}$, (b) $T = 0.5\,\text{keV}$ and (c) $T = 1\,\text{keV}$. Dashed lines: Rutherford theory,[1] dotted lines: experiments from Katase *et al.*,[19] dot-dashed lines: experiments from Danjo and Nishimura;[20] solid lines: present results by using the mean cross section based on the Mott model.[14]

In Eq. (12) the quantity $\text{Im}[-1/\varepsilon(q,E)]$ is commonly referred to as the energy loss function (ELF). We evaluate the ELF by using the method of Emfietzoglou *et al.*,[12] where the new optical-data model with the so-called 3D extend was presented.

The inelastic scattering angle θ_p of the primary electron and the ejection angle θ_s of the secondary electron are obtained by the empirical formulas.[24]

In addition, the azimuthal angle ϕ_p of the inelastic scattering of the primary electron is assumed to be uniformly distributed between zero to 2π, and the azimuthal angle ϕ_s of the secondary electron is taken as $\pi - \phi_p$.

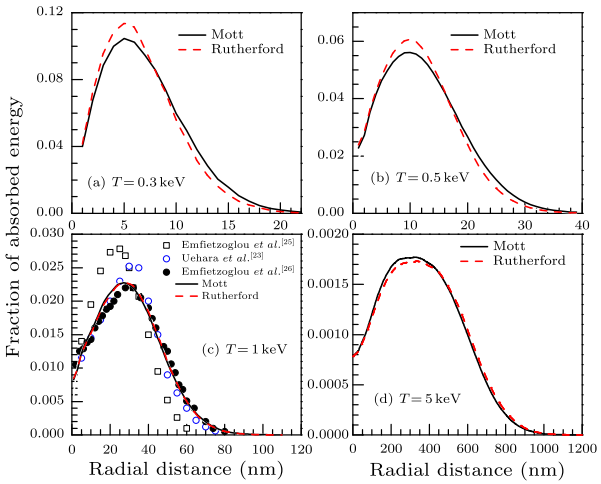

Fig. 3. Comparison of spatial distributions of energy deposition as a function of radial distance r at (a) $T = 0.3\,\text{keV}$, (b) $T = 0.5\,\text{keV}$, (c) $T = 1\,\text{keV}$, (d) $T = 5\,\text{keV}$.

With the use of the models described in this work, we have performed the calculations of both the spatial distributions of energy deposition of low-energy electrons and the electron penetration parameter in liquid water. In the simulations, liquid water is divided into a series of spherical shells at Δr intervals from the track origin, all the electrons, the primary and secondary electrons, are followed down to 10 eV in order to compare the simulation results with other theoretical calculations, and the number of the trajectories simulated is from 10^4 to 10^5 for obtaining good statistics.

The energies deposited in spherical shells are normalized to the total energies of the tracks, i.e. the so-called fraction of absorbed energy, for representing the spatial distribution of energy depositions. Figure 3 presents the calculated fraction of absorbed energy versus radial distance r at energies 0.3, 0.5, 1.0 and 5 keV. From Figs. 3(a) and 3(b), it can be seen that at 0.3 and 0.5 keV the difference between the results by the two elastic scattering models is obvious and that the Mott model produces evidently small energy absorptions in the radial region around peak positions when compared to the Rutherford formula and the reverse is true for large radial range. Figure 3(c) gives the comparison between the present results and other theoretical calculations from Uehara *et al.*[23] and Em-

fietzoglou *et al.*[25,26] Uehara *et al.*'s results are for water vapour. From Fig. 3(c), it is clear that the fraction of absorbed energy from Emfietzoglou *et al.*[25] displays the distribution range smaller than the others and it can also be seen that at 1 keV the distributions of the energy depositions from the two elastic scattering models are almost identical. In addition, as indicated in Fig. 3(c) the distributions of absorbed energy from Emfietzoglou *et al.*[26] are in good agreement with the present calculations. In Fig. 3(d), at 5 keV the Mott model leads to slightly large energy absorptions around peak position, in contrast with those by the Rutherford formula, and the reverse can be seen in a large radial range.

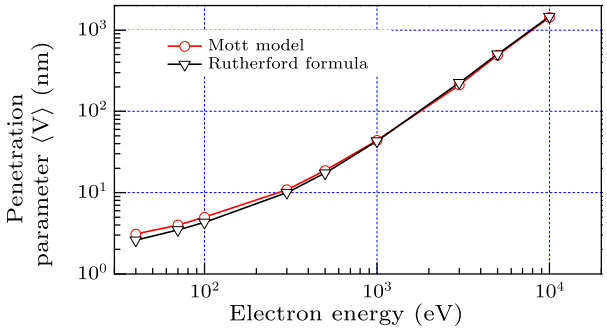

Fig. 4. Penetration parameter $\langle V \rangle$ as a function of incident electron energy.

As shown in the above analyses, relative to the absorbed energies by the Rutherford formula, the absorbed energies due to the Mott model exhibit the reverse change in the energy range below about 1 keV, when compared with those for the energy region above about 1 keV. However, the reason for this is not clear and should be further explored because of the complicated slowing-down process of energetic electron in liquid water.

By means of Monte Carlo calculations, many studies[13,27] have examined the energy dependence of the penetration range of low-energy electrons in liquid water. In this work, we have simulated the penetration parameter $\langle V \rangle$ of low-energy electrons in liquid water, where V is defined as the distance of the most distant transfer point relative to the starting point and $\langle V \rangle$ is the mean value of V. Figure 4 compares the simulated $\langle V \rangle$ by using the Mott model and Rutherford formula, respectively. The results of $\langle V \rangle$ due to the Mott model are smaller than those from the Rutherford formula within 3% in the energy range from 10 keV down to about 1 keV. At about 1 keV, $\langle V \rangle$ by the Mott model becomes larger, compared to the result from the Rutherford formula, and this discrepancy increases with the decreasing energy, bringing about an uncertainty up to about 13% at 40 eV. The reason producing this discrepancy may be attributed to the Rutherford cross sections larger than those from the Mott model at energies below about 1 keV, as shown in Fig. 1, because larger cross sections will result in smaller mean free paths and thus smaller $\langle V \rangle$.

In summary, we have investigated the influence of two fundamental models of electron elastic collision, i.e. the Rutherford formula and the Mott model, on the Monte Carlo simulation of low-energy electron transport in liquid water. Using the Monte Carlo code constructed in this work we have performed the systematical calculations of both the distributions of energy depositions and the penetration parameters for low-energy electrons in liquid water at different energies. The calculated results show that the influence of the two models becomes evident at energies below about 1 keV.

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