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Inelastic Mean Free Path and Stopping Power of Electrons in Bio-materials

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2. Keywords

1. Abstract

The inelastic mean free path and stopping power in organic and inorganic compounds are investigated and calculated using Drude dielectric formation. The minimum values of inverse mean free path λ^{-1} for organic and inorganic compounds at energy transfer ≈ 100 eV, while λ^{-1} distinguishable with previous work of Ashely (1988) and Garcia (2017). In the present work, exchange effects function f_{ex} (k) in the electron – electron interaction which is due distinguishability of scattered and ejected electrons. At low energy transfer SDCS, and $d\sigma/d\omega$ are independent of incident electron energy, while at $\hbar\omega \geq 10$ eV inversely proportional with incident electron. At Bragg`s peak ≈ 23eV, $d\sigma/d\omega$ is proportional with energy $E = \hbar\omega$ in power form.

3. Introduction

The transition of electrons through this a material must be well distinguished, so theoretical appreciations to know quantitatively how charged particles behave when movable through such material are wanted (Behar et al 2009) [1]. By the inelastic excitations of the target electrons the interaction of charged projectiles with material is influence through such the swift incident particles. In fact, these procedures are main exporter of slowing down for fast charged particles. Many techniques and applications need to know the energy loss of the project for quantitative purposes. (Denton et al 2008) [2].

Because the electron having rest mass, m, is very small in comparison with heavy charged particle masses, make up the main difference between heavy charged particle beams and electron beams occur. Incident electrons interacting with atomic electrons of the irradiated material can lose a large fraction of their energy in a single interaction. Heavy charged particles with mass M colliding with electrons will lose only a small fraction of their energy per collision (usually about 25 eV, but on the average 100 eV and at most $\approx 4mE/M$). When compared to electron beams, the heavy charged-particle beams have a smaller scattering angle and therefore have much sharper lateral distributions as they transverse a dense medium (Fadanelli et al 2015) [3].

The main objective of this work is to investigate the influence of the theoretical model for the Energy Loss Function (ELF) on the calculated (IIMFP), Single Differential Cross Section (SDCS) and Stopping power (S), Using the Drude model for describing response of the media to a perturbation, This model is based on more good theoretical arguments and reproduces experimental findings (Cruz and Yubero 2007) [4].

We have performed a systematic evaluation of IIMFP using the Drude model of ELF described for a large set of compounds (H_2O, DNA ($C_{20}H_{27}N_7O_{13}P_2$), PMMA ($C_5H_8O_2$), Adenine ($C_5H_5N_5$) and Guanine ($C_5H_5O\ N_5$)). In present work, a theoretical estimation of the stopping power and inelastic mean free path for incident electron in five compounds obtained using the Drude formula. As well as, we have also evaluated these magnitudes using two different approaches: (i) computations based of the dielectric formula, using exchange function f_{exch}, and (ii) Ashely (1988) presentation to a proper characterization of the electronic properties of the compounds at energies (10-104) eV. Good agreement achieved with previous work.

We show calculations, of the cross section (SDCS) in a wide incident electron energy range. Beside their substantial value, these results serve to validate theoretical foretelling for the energy loss and the mean-free paths of electrons in five compounds, but regrettably up to now, there are no experimental results to be compared to.

4. Theory

4.1. Dielectric Function

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Because of the technological attention of five compounds for integrated devices, the transmission of electrons through must be distinguish, so theoretical assessment to know quantitatively how charged particles behave when moving through this material are wanted. In particular, the inelastic energy loss of electron beams is pertinent since electrons are the projectiles utilized in several surface spectroscopy techniques (Went and Vos 2008) [5].

In order to obtain a very exact description of the electron energy loss processes, of the Stopping Power (SP), and of the inelastic mean free path (λ_{elect}), righteous even when electron energy is low, it is needful to consider the response of the ensemble of conduction electrons to the electromagnetic field created by the electrons passing through the solid: by a complex dielectric function this response is described. Ritchie theory, elucidate in particular, that the energy loss function, $\eta(\omega, k)$, necessary to compute both the (SP) as well as the inelastic mean free path, is the reciprocal of the imaginary part of the dielectric function $\eta(\omega, k)$ (Dapor et al 2013) [6],

$$\eta(\omega, k) = \text{Im}\left[-\frac{1}{\varepsilon(\omega, k)}\right] \tag{1}$$

$$\eta(\omega, 0) = \frac{a(Z_2)E}{[E^2 - b(Z_2)^2]^2 + c(Z_2)^2 E^2} \tag{1'}$$

Let us consider a superimposition of free and bound oscillators. In such case the dielectric functions, (Nikjoo et al 2013) [7].

$$\varepsilon(\omega, 0) = 1 - \omega_p^2 \sum_n \frac{f_n}{\omega^2 - \omega_n^2 - i\gamma_n \omega} \tag{2}$$

ω_p: is the plasma frequency

f_n: Are the fractions of the valance electrons bound with energies $\hbar\omega_n$

ω_n: Natural frequencies

γ_n: Are positive frictional damping. The extension from of dielectric function is:

$$\varepsilon(\omega, k) = 1 - \omega_p^2 \sum_n \frac{f_n}{\omega^2 - \omega_n^2 - \omega_k^2 - i\gamma_n \omega} \tag{3}$$

In the determination of the dispersion relating one has to take into account a constraint, known as the Bethe ridge. According to the Bethe surface, as $k \to \infty$, $\hbar\omega_k \to \hbar^2 k^2 / 2m$. Another way according $\omega_p^2 = 4\pi n e^2 / m$.

Ritchie (1957; 1991), present the following Eq.,

$$\hbar^2 \omega_k^2 = \frac{3E^2 v_f^2 k^2}{5} + \frac{E^4 k^4}{4m^2} \tag{4}$$

v_f: represent Fermi velocity, m: the electron mass,

Therefore Drude function becomes,

$$\eta(\omega, k) = \sum_n \frac{A_n \gamma_n \omega}{[\omega_n^2(k) - \omega^2]^2 + \omega^2 \gamma_n^2} \tag{5}$$

4.2. Inverse inelastic mean free path for electron λ_{elect}^{-1}:

The electron inelastic mean free path (IMFP), which represents the average distance between successive inelastic collisions, is one of the pertinent physical quantities for a quantitative analyse in electron-beam techniques like electron microscopy, x-ray photoelectron spectroscopy (XPS), or Auger electron spectroscopy (AES), among others (Garcia et al 2017) [8]. As well, electron IMFP is essential in the modeling of electron transport through solids and liquids (Dapor 2014) [9].

These relationships have then led us to general IMFP formula which we propose for use with other materials. Specifically, the new formula is considered useful for determining the IMFP dependence on electron energy for a particular material and the IMFP dependence on material for a given energy. Since al measurements of the needed accuracy are difficult, a formula is suggested as a reasonable but more approximate guide to (Tanuma et al 1987) [10].

When using an electron as a projectile, the key magnitude of interest is the inverse inelastic mean free path of electron (Werner 2004) [11]. The IIMFP, , λ_{elect}^{-1}, is a fundamental quantity to describe the electronic interactions of energetic electrons with biological compounds, because it is a measuree of the interaction vigor or the microscopic total cross section for electronic excitations and ionization operations of the target, gotten by $\sigma = 1/(N\lambda_{elect})$, where N is the density of scattering centers (Emfietzoglou et al 2013) [7]. Once the energy loss function has been gained, the differential inverse inelastic mean free path can be computed as (Yubero and Tougaard 1992) [26],

$$\frac{d\lambda_{elect}^{-1}}{d\omega} = \frac{1}{\pi T a_s} \int_{k-}^{k+} \frac{dk}{k} \eta(k, \omega) \tag{6}$$

$$k_{\pm} = \sqrt{2m\omega} \mp \sqrt{2m(\omega - \hbar\omega)} \tag{6'}$$

(Sabin and Oddershede 2005).

T is the incident electron energy

a_s, m and E are Bohr radius ~ 0.529 $\overset{\circ}{A}$, the electron mass and, transfer energy E = $\hbar\omega$

In other word Ashely (1988) define the electron differential inverse

inelastic mean free path $\frac{d\lambda^{-1}}{d\omega}$,

$$\frac{d\lambda^{-1}(\omega,E)}{d\omega} = \frac{me^2}{2\pi\hbar^2 T}\,\eta(\omega,0)L_e\left(\frac{\omega}{T}\right) \quad (7)$$

And the inverse inelastic mean free path is:

$$\lambda^{-1}_{eloct} = \frac{1}{\pi T a_e}\int_{k_-}^{k_+}\frac{dk}{k}\,\eta(\omega,k)\int_0^{W_{max}} d\omega \quad (8)$$

The inverse inelastic mean free path λ^{-1}_{eloct} of electrons penetrating solid targets (Garcia et al 2017) present by Ashely present by Ashely (1991)

$$\lambda^{-1}_{eloct}(E) = \frac{me^2}{2\pi\hbar^2 T}\int_0^{W_{max}}\eta(\omega,0)\,L_e(\omega/T)\,d\omega \quad (9)$$

And $W_{max} = T/2$, is the maximum energy loss (see Ashley 1991) for dielectric details with e the electron charge and with $\hbar$ the Planck constant h divided by 2π).

Ashley (1988) explains a good approximation of the function L(x) is getting by:

$$L(x) = (1-x)\ln\left(\frac{4}{x}\right) - \frac{7}{4}x + x^{3/2} - \frac{33}{32}x^2 \quad (10)$$

$x = \omega/E$ in Eq. 9

At large energy, i.e x<<1, Eq.(10) approximated to,

$$L_e(x) \approx \ln\left(\frac{4}{x}\right) - \frac{7}{4}x - \frac{33}{32}x^2 \qquad x \ll 1 \quad (10^`)$$

There is an exchange effects in electron-electron interaction due to indistinguishably of incident (scatted) and ejected (target) electrons,

The maximum energy transferred in a collision will be $\hbar\omega = mv^2/4$, since the incident electrons are the most energetic after the collision. The exchange effect between incident and target electrons represent by the following function (Dapor et al 2015).

$$f_{exchange}(k) = 1 + x^2(k)(x^2(k)-1), \quad (11)$$

Where $x(k) = (\hbar k/mv)$

Rewrite Eq. (8)

$$\lambda^{-1}_{eloct} = \frac{1}{\pi T a_e}\int_0^{W_{max}} f_{exchange}\frac{dk}{k}\,\eta(k,\omega)\,d\omega \quad (12)$$

4.3. Single Differential Cross Section of SDCS (Incident Electron)

As energetic electrons cross through matter they lose energy primarily through collisions with bound electrons. Ionization cross sections for all primary and secondary electrons are needed to follow the history of an incident particle and its products, covering all ranges of energy transferred in individual collisions (Nikjoo et al 2016) [14]. The single differential cross section (SDCS) for ionization of i-shell electrons by a electrons with kinetic energy T is given in Eq. (7)

The macroscopic cross section is attached to the microscopic cross section σ, by the relation,

$$\lambda^{-1} = N\sigma, \quad (13)$$

$$\frac{d\lambda^{-1}}{d\omega} = N\frac{d\sigma}{d\omega} \quad (14)$$

Substitute Eq. (7) into Eq. (15)

$$\frac{d\sigma}{d\omega} = \frac{1}{N}\frac{d\lambda^{-1}}{d\omega}$$

$$= \frac{me^2}{\pi\hbar^2 T}\frac{1}{N}\int_{k_-}^{k_+}\frac{dk}{k}\eta(\omega,0) \quad (15)$$

Therefore, total integrated inelastic cross-section is obtain by integration (15)

$$\sigma(T) = \int_0^{\omega_{max}}\frac{d\sigma(T)}{d\omega}\,d\omega,$$

$$= \frac{me^2}{\pi\hbar^2 T}\frac{1}{N}\int_0^{W_{max}}d\omega\int_{k_-}^{k_+}\frac{dk}{k}\eta(\omega,0)d\omega \quad (16)$$

With $w_{max}=T/2$,

In atomic unite, with $\hbar=m=e=1$, Eq. (16) becomes,

$$\sigma(T) = \frac{1}{\pi T N}\int_0^{W_{max}}d\omega\int_{k_-}^{k_+}\frac{dk}{k}\eta(\omega,0) \quad (17)$$

$$W_{max} = v^2/4$$

Eq. (7) required the contribution of each the electronic shell of the target to its energy loss function, and the latter is measure for the excitations and ionizations of the electronic system in the optical limit (k=0), the algorithm to obtain the data at k>0 and splitting this energy loss function into different electronic shells is needs in addition to experimentally measured ELF. The optical energy loss functions of bioorganic condensed compounds and water which are similar and can be parameterized with single Drude formula by using (Eq.1`). The differential inelastic cross section $d\sigma/d\omega$, that can be numerically obtained from experimental optical data to

obtain accurate electron energy spectra and total ionization cross sections (TICS) for ion impact in arbitrary condensed biological materials, by only knowing their atomic composition and density (de Vera et al 2015) [15].

4.4. Stopping Power of Electron

The stopping power (s.p) (also purport stopping force) for electron is a quantity of fundamental importance to hadron therapy and biophysics (Nikjoo et al 2008) [16]. Although a significant amount of work has been concerned with electron mean free paths, rather less is available on stopping powers for electrons with energies range (10-104) eV. A summary of stopping power calculations is given in (Tan1 and Tan2 et al 2004) [17, 18]. A main feature of this paper is to provide a simple method for evaluating electron energy loss per unit path length in this low-energy region from available optica006C data.

For an energetic ion interacts with a medium having kinetic energy T , mass m , atomic number z and charge, whose electronic excitatio spectrum is illustrate by its energy loss function Im[-1/$\varepsilon(k,\omega)$], the target (s.p) $(-dE/dx)$ can be performed by (Dapor 2014) [9].

$$-\frac{dE}{dx} = \frac{me^2}{\pi\hbar^2 T}\int_0^{W_{max}} \eta(\omega,0)\, S(\omega/T)\, d\omega$$

(19)

Besides, the indistinguishability between the incident electron and a generated secondary electron means that the maximum energy transfer cannot exceed T/2.

Where a simple expression can be get by expanding the analytic functions resulting from the ω integration in powers of ω/T. Through second order terms in ω/T, we find (Ashley 1988) [19]:

$$S(x) = \ln\frac{1.166}{\varepsilon} - \frac{3}{4}x - \frac{\varepsilon}{4}\ln\left(\frac{4}{x}\right) + \frac{1}{2}x^{3/2} - \frac{x^2}{16}\ln\left(\frac{4}{x}\right) - \frac{31}{48}x^2$$

(20)

To compute the (s.p) from Eq. (19), we need a suitable characterization of the energy-loss function ELF of the target, Im[−1/$\varepsilon(0,\omega)$] . We applied the Drude model energy loss function to describe the ELF of four compounds and liquid water since it has been successfully utilized to depict the ELF of materials with a complex electronic spectrum. The outer- and inner-shell electrons Contributions to the excitation spectrum which are treated separately accordingly the following expression. Let us now consider the collisions with the stopping medium resulting in a kinetic energy transfer from the projectile to the target atoms and/or molecules constituting the target. Let us assume that the energy transfer E_i (10-10⁴) eV is small with respect to the incident particle kinetic energy T.

Finally, the exchange effects in the electron –electron interaction due to the indistinguishability of scatted and ejected electrons must be deemed when the energy of both electrons are similar. Therefore integrate Eq. 6 over ω, taking function $f_{exch}(\hbar k/mv)$, in the consideration,

$$\left(-\frac{dE}{dx}\right) = \frac{1}{\pi T a_0}\int_{k-}^{k+}\frac{dk}{k}\int_0^{W_{max}} \eta(\omega,0)\, f_{exch}(\hbar k/mv)\, \omega\, d\omega$$

(21a)

Where f_{exch} is defined in Eq. (11) and $k_{\pm}$ are defined in Eq. (6). $T = 1/2\, mv^2$, with Bohrs radius $a_0 = 2\hbar/me^2$, therefore Eq. (21a) becomes,

$$\left(-\frac{dE}{dx}\right) = \frac{me^2}{\pi\hbar^2 T}\int_{k-}^{k+}\frac{dk}{k}\int_0^{W_{max}} \eta(\omega,0)\, f_{exch}(\hbar k/mv)\, \omega\, d\omega$$

(21b)

In the present work, Drude formula have been used to analyse the stopping power calculations of different complex organic compounds Liquid water, DNA $C_{20}H_{27}N_7O_{12}P_2$, PMMA (Poly(methacrylates): $C_5H_8O_2$, Adenine: $C_5H_5N_5$, and Guanine: $C_5H_5N_5O$.

5. Results and Discussion

Fig. (1) shows the electronic mean free path λ_{elect} for electrons in (a) Liquid water, (b) DNA, (c) PMMA, (d) Adenine and (e) Guanine as a function of electrons kinetic energy $T = mv^2/2$ in eV for two different models, present work using Ashley (1988) and present work including exchange function, f_{exch}. They are agree at energy $T \approx 100\, eV$, while at T<100 eV and at high energy T>100 eV there is discrepancy between them. Fig (1) explain mean free path for incident electron by using Eq. (9, 12) and programmed them in Khalaf 2018 [20]. Good agreement achieved with available work of PMMA (Dapor 2014) [9], for Guanine (Tan1 &2 2004) and for DNA (Garcia et al 2017) [8].

As a result of the energy delivered by a fast electron along its path, secondary electrons are emitted as a result ionization of the target atoms. These electrons move away from the region where they generated, experiencing elastic and inelastic scattering with the target components, losing energy through excitations and producing new ionizations, which results in an avalanche of electrons and is the standard procedure to obtain elastic IMFP for electrons (Dapor et al 2017) [12]. However, it should be kept in mind that due to the electron energies involved in this work, no relativistic corrections are required in the electron kinematics.

Fig. (2) Shows the single differential cross section (SDCS), $d\sigma/d\omega$ in (A²/eV) with energy transfer $E = \hbar\omega$ in eV. The SDCS`s for ionization of (a)Liquid water, (b) DNA, (c) PMMA, (d) Adenine, (e)

Guanine by electrons of a given energy (T_e=0.001-0.005) Mev with energy transfer $E = \hbar\omega$ in eV which they are typical projectile energies and Bragg peak as shown in fig. (2). One can see that the single differential cross section $d\sigma/d\omega$ of electrons decrease when the incident electrons energy increases, meaning that the largest ionization at Bragg`s peak. The other point $d\sigma/d\omega$ decreases with increasing $T_e$ this is due to time of interaction decreases as well. SDCS $d\sigma/d\omega$ varies with incident electron energy, at $T_e$ Bragg`s peak as follows,

$$\frac{d\sigma}{d\omega} = a \ E_{Brag}^{-b}$$

(22)

Where $E_{Bragg} \approx$ 23 eV. Table (1) shows the SDCS, $d\sigma/d\omega$ in (A^2/eV) at different incident electron energy T_e in Mev.

In Table (2) show the SDCS parameters a and b given in Eq. (18) of five compounds with electron incident energy in MeV with range (0.001-0.005).

When incident electron energy in the region of ($1-10^4$) eV we note Adenine and Guanine having the large value in stopping power is (33) eV/nm for Adenine and 35 (eV/nm) for Guanine as shown in fig. (3).

Fig (3) shows the stopping power in (eV/nm) takes f_{exch} in the consideration, Eq. (21b) and from Ashely (1988) model, Eq. (19) with energy transfer in eV. For Liquid water and four organic compounds DNA, PMMA, Adenine and Guanine. At energy $T \leq 100\ eV$ there is no different between present works with f_{exch} and Ashely model. The maximum difference between them the energy >100 eV $\approx$ 45% at Braggs peak as shown in fig. (3) show the biggest value for Guanine and Adenine because two compounds have large density.

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