

Shell Correction in Stopping Power for Protons with Different Ionization Degrees in Al_2O_3 and ZrO_2

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Abstract. The shell correction and stopping power of Aluminum oxide Al_2O_3 and Zirconium oxide ZrO_2 for protons over the 10 KeV to 10000 KeV energy range is studied using an improved Drude dielectric function. In present work the effects of charge fraction on the stopping power and shell correction has been taken in the consideration and investigated. The main point is to get more information about the energy loss function ELF of compounds Al_2O_3 and ZrO_2 , which is important in studying the stopping power of protons. The shell correction is one of the corrected term to Bethe formula give more attention to compounds is converging at high energy $E \geq 700 keV$ and increasing at incident proton energy $0 \leq E(keV) \leq 700$ Good agreement is achieved with previous work.

1. Introduction

Alumina Al_2O_3 and Zirconium ZrO_2 are an important material broadly used in mechanical, optical, optoelectronics or microelectronic applications. They are a typical choice as a matrix/substrate for optical waveguide amplifiers in integrated systems, solid state lasers or thin-film devices [1,2]. The investigation of energy deposition of energetic ions in matter is important and problem of interest for applied research if different source of area like ion implantation, ion beam analysis and modification of materials, radiation damage, radiation therapy and space research [3-5]. Modified Drude formula [1] of dielectric function has been used to calculate the energy loss function $\text{Im}\left[-\frac{1}{\epsilon(k, \omega)}\right]$. The stopping power of proton beams in Al_2O_3 and ZrO_2 were studied by previous work [6-8].

In the present work we also calculate and studied the shell correction $(-C/z_2)$ for proton beam in Al_2O_3 and ZrO_2 taking in the consideration charge exchange.



2. Theory and discussion

Suppose a swift projectile of mass M_1 , atomic number Z_1 , kinetic energy T and charge q moves inside materials, it induces electronic excitations inside the material, losing energy in the process. The probability per unit path length $P_q = (T, E)$ that the projectile with charge state q and energy T produces in the target an excitation of energy $E = \hbar\omega$ is given by [9]:

$$P_q(T, E) = \frac{M_1 e^2}{\pi \hbar^2 T} \int_{k_{\min}}^{\infty} \frac{dk}{k} \rho_q^2(k) \int \text{Im} \left[\frac{-1}{\varepsilon(k, \omega)} \right] \quad (1)$$

$$\text{Where, } k_{\min} = \omega / 2T / M_1,$$

$\rho_q(k)$ is Fourier transform of the projectile charge state density presented by Brandt and Kitagawa BK [10,11] :

$$\rho_q(k) = Z_1 \frac{q + (k\Lambda)^2}{1 + (k\Lambda)^2}, \quad (2)$$

Where Λ is a variation parameter given by:

$$\Lambda = \frac{0.48 N^{2/3}}{Z_1 - N/7}, \quad (3)$$

With N is the number of bound electrons and $q = 1 - N/Z_1$ is the charge fraction. Integrating equation (1) over energy transfer $E = \hbar\omega$ gives the stopping power of the projectile $S(q)$ [9],

$$S_q(v) = \frac{M_1 e^2}{\pi \hbar^2 T} \int_{k_{\min}}^{\infty} \frac{dk}{k} \int_0^{kv} \omega d\omega \rho_q^2(k) \int \text{Im} \left[\frac{-1}{\varepsilon(k, \omega)} \right] \quad (4)$$

Equation (4) gives the average energy loss per unit path length, as the weighted sum of the stopping power of different charge state q that the projectile travels through the target. That is [9]:

$$S(v) = \sum_{q=0}^{\infty} \phi_q(v) S_q(v) \quad (5)$$

ϕ_q is the fraction of charge state q and $S_q(v)$ is the corresponding stopping power at velocity v , and the sum over all possible charge state q of the projectile ϕ_q . Satisfy the normalization

condition $\sum_{q=0}^{Z_1} \phi_q(v) = 1$ and a detail for calculation of ϕ_q is given in [1].

The inelastic collisions of projectile with target can be described by energy loss function ELF within formalism given in equation (4). There are different kind of response of the target, valence-

band, *vb* and inner shell, *ish* electrons to the perturbation induced by the projectile charge. Therefore we assume that:

$$\text{Im}\left[\frac{-1}{\varepsilon(k, \omega)}\right] = \text{Im}\left[\frac{-1}{\varepsilon(k, \omega)}\right]_{vb} + \text{Im}\left[\frac{-1}{\varepsilon(k, \omega)}\right]_{ish}, \quad (6)$$

Where $\text{Im}[-1/\varepsilon(k, \omega)]_{vb}$ and $\text{Im}[-1/\varepsilon(k, \omega)]_{ish}$ are the contribution of ELF due to valence-band and inner-shell electrons respectively,

$$\text{Im}\left[\frac{-1}{\varepsilon(k, \omega)}\right]_{vb} = \sum_i \frac{A_{Di} \nu_i \omega_i}{\{\omega_i^2(k) - \omega_i^2\}^2 + (\nu_i \omega_i)^2} \theta(\omega_i - \omega_{th,i}), \quad (7)$$

Where A_{Di} , ω_i , ν_i and $\omega_{th,i}$ are the intensity, position, width and threshold respectively of Drude-ELF peaks. $\theta(\dots)$ represent the Heaviside step function [9].

$$\omega_i(k) = \omega_i + g(k) \frac{k^2}{2m}, \quad (8)$$

$$g(k) = 1 - \exp(-ck^d), \quad (9)$$

$$\nu_i(k) = \nu_i + ak + bk^2. \quad (10)$$

$$a = 10eV, \quad b = 6eV, \quad c = 1.2 \text{ and } d = 0.4$$

$$\text{Im}\left[\frac{-1}{\varepsilon(k, \omega)}\right]_{ish} = \frac{2\pi N_m}{\omega} \sum_j \alpha_j \sum_{nl} \frac{df_{nl}(k, \omega)}{d\omega} \quad (11)$$

Where N_m is the molecular density of the target (molecular per unit volume) and $df_{nl}(k, \omega)/d\omega$ is the generalized oscillator strength GOS of the (n, l) subshell of the j th element. The sum over the inner shells of all atoms in the compound [1].

3. Results and discussion

Shell correction is the most important correction to Bethe formula especially below 1MeV proton energy. The correction is due to the dipole approximation and leads to ionization potential. The shell correction $(-C/Z_2)$ follows Bethe formula as follows [12]:

$$S_{Bethe} = \frac{z_1^2 E_p}{2T} \left[\ln\left(\frac{4T}{I}\right) - \frac{C}{z_2} \right] \quad (12)$$

Fano (1963) gives an expression of shell correction, which contributes of each individual shell. In terms of ELF, Fano's expression reads [12]:

$$\frac{C}{z_2} = \frac{C_1}{z_2} + \frac{C_2}{z_2}, \quad (13)$$

$$\frac{C_1}{z_2} = \frac{2}{\pi E_p^2} \int_0^{E_{\max}} \omega d\omega \int_0^{k_{\min}} \frac{1}{k} \left\{ \text{Im}\left[\frac{-1}{\varepsilon(\omega, k)}\right] - \text{Im}\left[\frac{-1}{\varepsilon(\omega, 0)}\right] \right\} dk, \quad (14)$$

$$\frac{C_2}{z_2} = -\frac{2}{\pi E_p^2} \int_0^{E_{\max}} \omega d\omega \int_{k_{\min}}^{\infty} \frac{1}{k} \text{Im} \left[\frac{-1}{\varepsilon(\omega, k)} \right] dk. \quad (15)$$

Since $k_{\min} = \omega/(2T/M_1)$ and $k_{\max} = \omega/v$, the shell correction term depends on incident proton energy. E_p is the nominal plasmon energy of the material determined from the relationship, $E_p = 4\sqrt{n\pi a_0^3} R_y$, n is the electron density and $R_y = 13.6\text{eV}$.

Figure (1) represents the optical limit ($k = 0$) of the present two target oxides materials (i.e aluminum oxide, and zirconium oxide, ZrO_2) for energy loss function ELF as a function of the excitation energy of the target electrons $E = \hbar\omega$ in eV

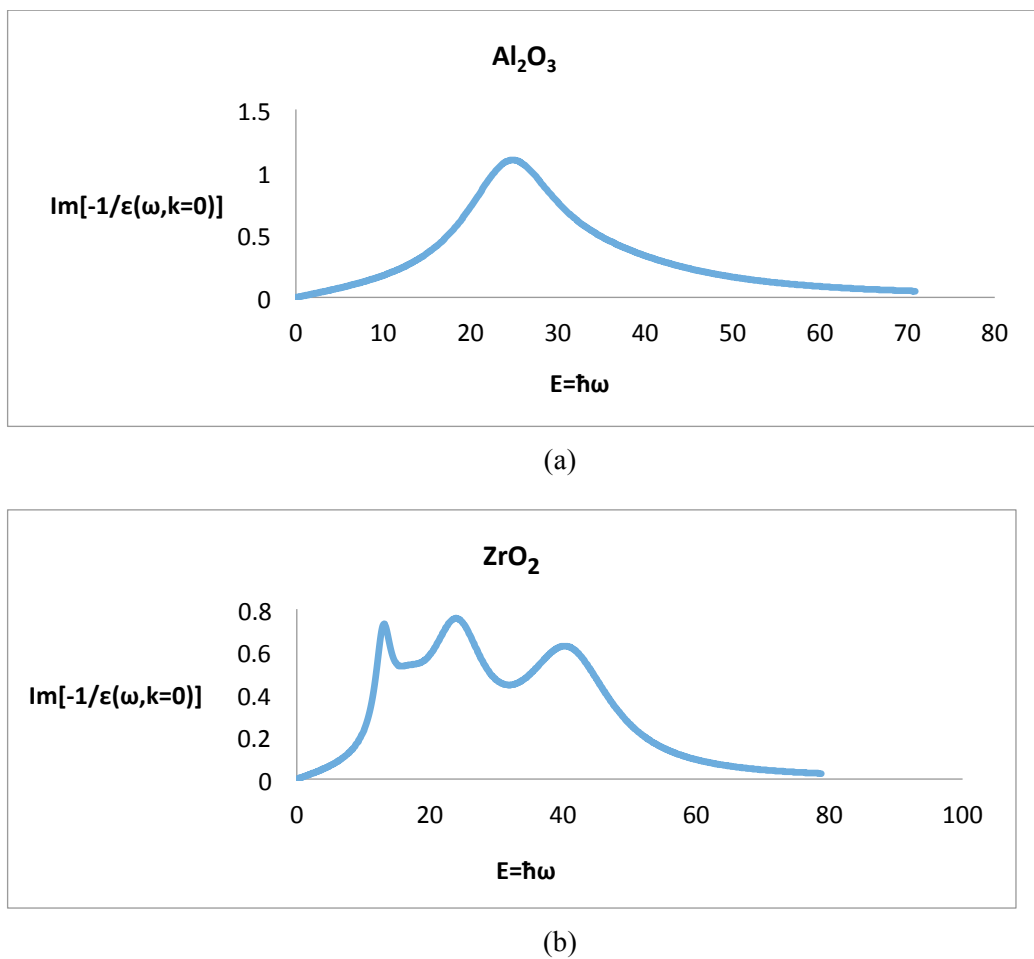


Figure 1. Two dimensions energy loss function $\text{Im}[-1/\varepsilon(\omega, k = 0)]$ with energy transfer $E = \hbar\omega$ in eV for (a) Al_2O_3 and (b) ZrO_2

For clarity we plot ELF at ($k = 0$) and its extension at $k > 0$ is represented in figure (2). The parameters used in describing ELF of Al_2O_3 and ZrO_2 has been taken from [9]. Good agreement achieved with previous experimental and theoretical results of ELF given in [9].

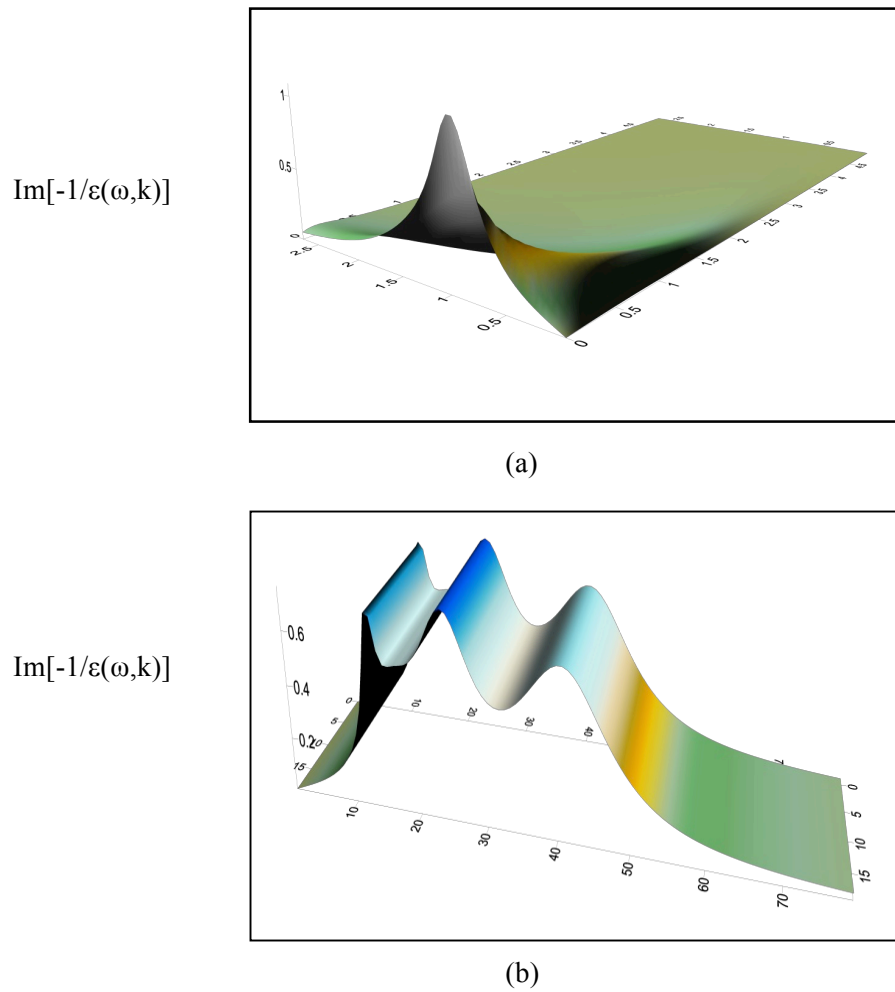
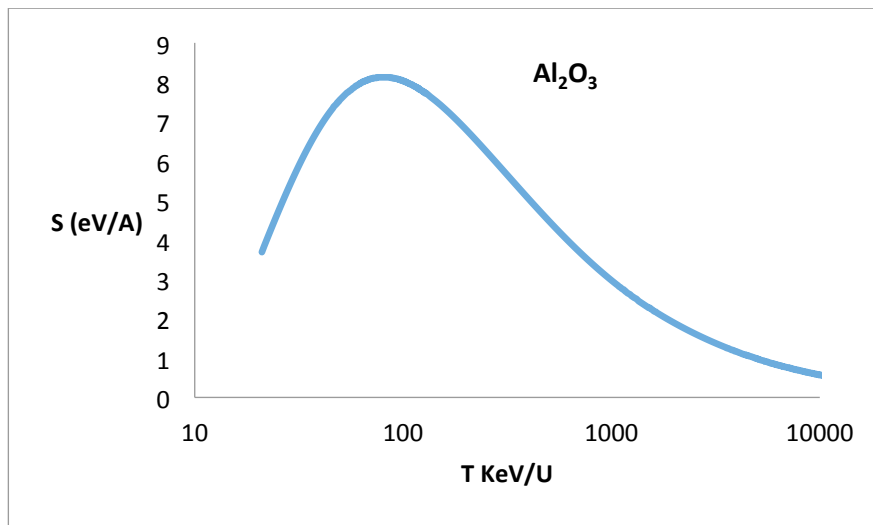
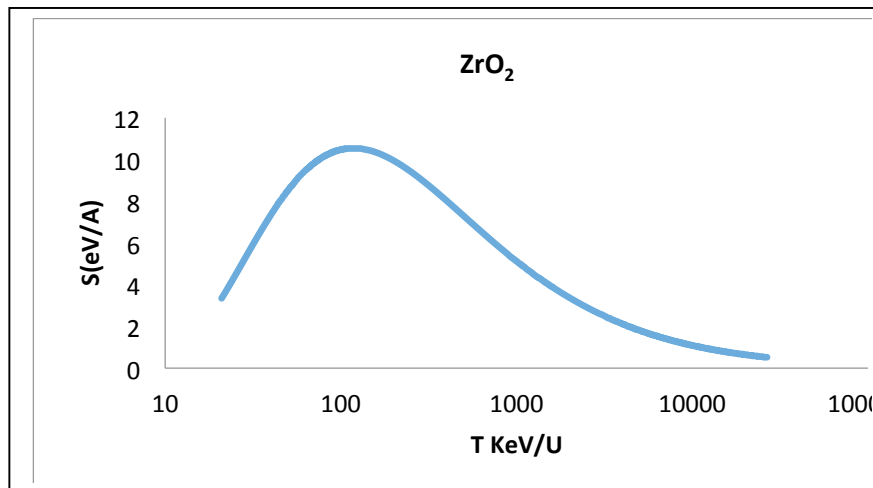


Figure 2. Three dimensions energy loss function $\text{Im}[-1/\varepsilon(\omega, k)]$ with energy transfer $E = \hbar\omega$ in eV for (a) Al_2O_3 and (b) ZrO_2

Using equations (1) and (5) with a previous representation of ELF for and ZrO_2 , the charge fraction density $\rho_q(k)$ for BK given in equation (2), we have calculated the stopping cross section SCSs, $S(\text{eV} / A^0)$ for protons in Al_2O_3 and ZrO_2 as a function of protons energy T in keV as shown in figure (3). The present results of stopping power $S(\text{eV} / A^0)$ are in good agreement with previous theoretical and experimental work given in [13] and prediction of SRIM- 2008 code [14]



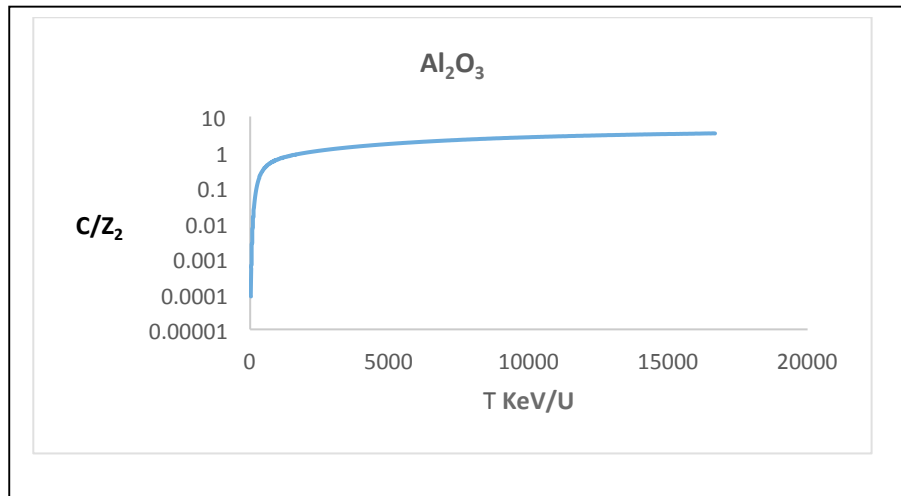
(a)



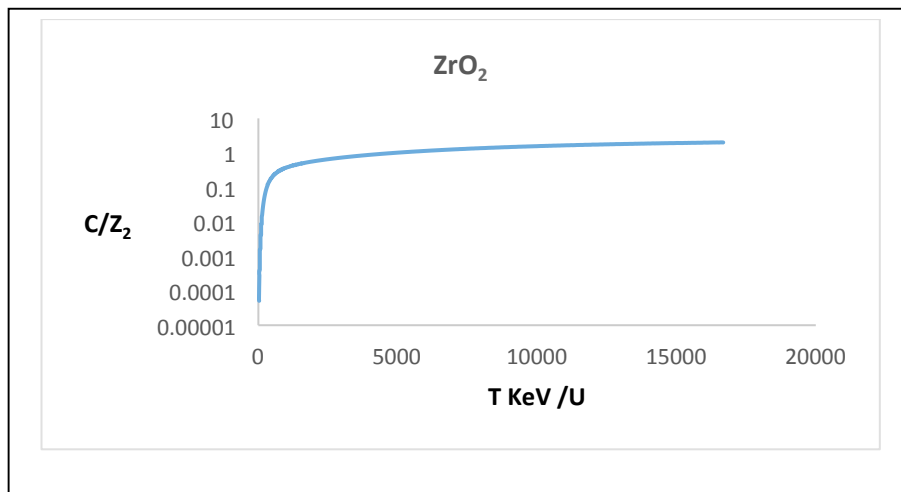
(b)

Figure 3. The stopping cross section of (a) Al_2O_3 and (b) ZrO_2 for swift proton as a function of their energy per atomic unit, T in KeV/u .

The shell correction (C/Z_2) defined as the difference between the Bethe and Born stopping numbers, equation (12) and by Fano's expression (equations (14) and (15)), while the present results of shell correction are shown in figure (4). There is no previous theoretical or experimental result of shell correction (C/Z_2) of proton in Al_2O_3 and ZrO_2 to compare with.



(a)



(b)

Figure 4. The shell correction (C/Z_2) calculated from the present response model using equations (13)-(15) of (a) Al_2O_3 and (b) ZrO_2 for swift proton as a function of their energy per atomic unit, T in keV/u

4. Conclusion

Energy loss function ELF plays an important role in calculating the stopping power and shell correction. The accuracy of parameters describing outer electrons to the ELF spectrum are important to specify ELF due to outer electrons and the generalized oscillator strength GOS for inner shell. The different in results of stopping power with SRIM output about $\approx 15\%$ for ZrO_2 and $\leq 10\%$ for Al_2O_3 . SRIM output of compounds comes from Bragg's additive rule which needs more work to do.

Using the optical data of ELF, $\text{Im}[-1/\epsilon(k=0, \omega)]$ the shell correction (C/Z_2) for proton in Al_2O_3 and ZrO_2 is shown in figure (4a, 4b). The shell correction $0 < (C/Z_2) < 1$ at low incident proton energy $E \leq 700keV$, and $(C/Z_2) \rightarrow 1$ at high incident proton energy $E > 700keV$ as shown in figure (4a, 4b).

5. References

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