Electron inelastic mean free paths in solids: A theoretical approach*

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In the present paper, the inelastic mean free path (IMFP) of incident electrons is calculated as a function of energy for silicon (Si), oxides of silicon (SiO_2), SiO, and Al_2O_3 in bulk form by employing atomic/molecular inelastic cross sections derived by semi-empirical quantum mechanical method developed earlier. A general agreement of the present results is found with the most of the available data. It is of great importance that we have been able to estimate the minimum IMFP which corresponds to the peak of inelastic interactions of incident electrons in each solid investigated. New results are presented for SiO for which no comparison is available. The present work is important in view of the lack of experimental data on IMFP in solids.

Keywords: electron inelastic mean free path, complex potential, inelastic electron scattering cross sections, solids

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1. Introduction

Inelastic mean free path (IMFP) of electrons passing through a medium has been a subject of long-standing interest in view of its important role in the physics of surface thin films and various solids. When external electrons interact with a bulk medium, the inelastic processes result in energy loss. Accurate scattering surface analysis by Auger electron spectroscopy and x-ray photoemission spectroscopy requires the IMFP which is also useful in determining surface sensitivity.[1] Energetic photons of radiation interacting with solids as well as living organisms liberate secondary electrons which can induce excitations and ionization, and other interaction processes can also occur depending on the impact energy. Matter in condensed forms is also presented in various solar-system objects (planets, the moon, asteroids with almost no atmosphere) and outer-space environments, and it is exposed to energetic electrons from sources like solar wind, etc. In short, the electron IMFP plays an important role in any experiment or a situation which involves motion of electrons through solids or condensed matters, and this includes as well the electron diffraction, Bremsstrahlung spectroscopy, and so on.

A comprehensive review and data base in the context of electron IMFP have been reported in Ref. [1]. The IMFP on the solid surfaces of various elements and compounds have been calculated by several authors.[2−8] Most of the IMFP data are obtained in the impact energy higher than 50 eV. The prevailing approaches in calculating the IMFP are broadly based either on low-energy method or on high-energy method. Ashley *et al.*[9−11] have calculated IMFP for many solids from optical data, using a variety of models[9−12] and have included the effect of damping, exchange and correlation, and ion-core polarizability with complex dielectric response function proposed by Lindhard,[13] from 40 to 10000 eV. Tung *et al.*[10,14] used electron-gas statistical model and calculated the IMFP for bulk Al, Si, Ni, Cu, Ag, and Au. The IMFP can be directly computed from experimental energy-loss functions of different materials as pointed out by Powell.[15] The IMFPs for C, Mg, Al, Al_2O_3, Cu, Ag, Au, and Bi in bulk have been calculated using this model in the energy range of 100–2000 eV, by employing Penn algorithm.[16] Tanuma *et al.*[17−20] have calculated in their TPP-2 model, the IMFPs of electrons for 56 materials comprising of elements together with inorganic and organic compounds, in the energy

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range of 50–2000 eV. A unified model prevailing down to low energy of electrons in diamond has been given by Ziaja *et al.*[21] However, we note that there are discrepancies among various results available in literatures on the same target, and in many cases the minimum of the IMFP as a function of incident energy is not clearly obtained.

In this backdrop, our effort in the present paper is based on a micro-to-macro approach. Specifically, we start with the electron impact total inelastic cross section from a target in a single scattering event, and then deduce the IMFP at intermediate and high electron energies. At low energies, the influence of various bulk processes prevails, whereas at high enough energy individual atomic/molecular scattering becomes meaningful. Presently we have tried to find the minimum IMFP of electrons in selected solids at intermediate to high energies with the help of a semi-empirical quantum mechanical approach developed by Joshipura *et al.*[22−27] In Refs. [22] and [28–30], the electron impact ionization of H_2O in condensed phases (ice and liquid) has been studied, and the formalism and calculated results of ionization as well as the inelastic mean free path in condensed matter have been provided. Various bulk processes such as electron–phonon scattering and vibrational excitation are not taken in to account in the present scattering model since these are mainly low-energy processes.

An attempt has been made here to estimate the electron inelastic mean free path ($\lambda_{\rm IMFP}$) for Si, SiO_2, SiO, and Al_2O_3 in bulk forms, with incident energy $E_{\rm i}$ ranging from ∼20 to 2000 eV. In the present theoretical model, total inelastic cross sections $Q_{\rm inel}$ of electron impact on the present (atomic/molecular) targets are determined with the complex scattering potential, in the framework of partial wave analysis. The variable phase approach used in our previous papers is employed.[22−27] A basic input in this calculation is the atomic/molecular charge density, which should be modified properly to account for the bulk or solid-state effects. Therefore, the charge density is constructed here, as have done in Ref. [25]. The Wigner–Seitz boundary conditions are used to approximate the realistic atomic charge distribution. The IMFP are calculated using the microscopic cross sections $Q_{\rm inel}$ as the key input, and calculated results are compared with available experimental and theoretical data except for SiO, where no data are available.

2. Theory and calculation

At appropriately high energy, the de-Broglie wavelength of the incident electron exceeds typical crystalline bond distances, and it becomes reasonable to consider single (atomic or molecular) scattering model for electron inelastic processes. For example, for an incident electron of 20 eV energy, the de Broglie wavelength is 2.74 Å, which is comparable to the crystalline bond distances. In addition, at low energies, the bulk (collective) excitations are expected to dominate. Therefore, the present scattering model approach is applicable for energy higher than 20 eV. With the present theoretical approach, we first focus on calculating total inelastic cross sections and treat the scattering problem in a spherical complex optical potential, $V(r, E_{\rm i}) = V_{\rm R} + {\rm i}V_{\rm I}$, that represents simultaneous elastic and inelastic scattering of electrons from the embedded target atom or molecule. The functions $V_{\rm R}$ and $V_{\rm I}$ are the real and imaginary parts of total potential V, and the imaginary part $V_{\rm I}$ accounts for all the accessible inelastic channels in the embedded target. The exchange and correlation effects are incorporated into the real potential term $V_{\rm R}$ as follows:

$$V_{\rm R} = V_{\rm st} + V_{\rm ex} + V_{\rm cp}, \tag{1}$$

where $V_{\rm st}$, $V_{\rm ex}$, and $V_{\rm cp}$ stand for the (attractive) static, exchange, and correlation polarization potentials of the target, respectively. The static potential $V_{\rm st}$ is calculated from atomic charge density $\rho(r)$, which is adopted by us from Salvat *et al.*[31] The atomic electron-charge density is the first input in our theoretical method, and is obtained for atom/molecule bound in condensed phase, by considering analytical expressions in Ref. [31]. When the target atoms are bound in a solid, the self-consistent field procedure is carried out under Wigner–Seitz boundary conditions to describe approximately the atomic charge distribution. The charge density obtained differs considerably from the free-atom case as reported in Ref. [31].

The imaginary part of the total complex potential $V_{\rm I}(r, E_{\rm i})$ accounts for cumulative inelastic scattering in accordance with energy and particle-flux conservation. For the interactions of electrons and atoms or molecules, the $V_{\rm I}$ is expressed as a local energy-dependent absorption potential $V_{\rm abs}$.[32] The absorption potential is constructed appropriately to account for all admissible channels of inelastic scattering. This absorption potential is based on the Mott scattering between the incident and the target electrons, and has

a generic form as follows:

$$V_{\rm abs} = -\rho(r)\left(\frac{T_{\rm loc}}{2}\right)^{1/2}\left(\frac{8\pi}{10k_{\rm F}^3 E_{\rm i}}\right) \times \theta(p^2 - k_{\rm F}^2 - 2\Delta)(A_1 + A_2 + A_3), \quad (2)$$

where $\rho(r)$ is the atomic or molecular charge density of the target, and $T_{\rm loc}$ is the local kinetic energy of the projectile electron in the target region. The function $\theta(x)$ is the Heaviside unit step function, and $\theta(x) = +1$ for $x > 0$, and zero otherwise. Furthermore, $p = \sqrt{2E_{\rm i}}$ is the incident momentum in atomic units, and $k_F = (3\pi^2\rho(r))^{1/3}$ is the corresponding Fermi wave vector. The local kinetic energy of the incident electron in the target region is given by

$$T_{\rm loc} = E_{\rm i} - (V_{\rm st} + V_{\rm ex}). \quad (3)$$

The quantity Δ in Eq. (2) is a crucial energy parameter which defines a threshold. If $E_{\rm i} \leq \Delta$, then

$$V_{\rm abs} = 0. \quad (4)$$

In this case, no excitation or ionization would take place.

In gas-phase calculations,[27] the energy parameter Δ is basically chosen to be at or near the ionization threshold I of the target, and the resulting calculations are found to exhibit a good general agreement with relevant data. In the case of Si atom, the threshold I =8.15 eV, which does not correctly determine the scattering mechanism in the condensed matter case. In the free or gas case, the incident or primary electron with energy slightly higher than the first ionization energy can ionize or eject a valence electron from the target, and both the scattered and ejected electrons can move out freely. In a condensed medium, the situation is quite complex. The ionization effectively takes place only if the incident energy $E_{\rm i}$ exceeds the ionization threshold I by an amount of the energy-band gap denoted by $E_{\rm gap}$.[33] In other words, the threshold energy parameter must be chosen to be $\Delta = I_{\rm Si} + E_{\rm gap} = 9.26$ eV, since $E_{\rm gap} = 1.1$ eV for metallic Si.[33]

Using this formalism, the inelastic cross section can be generated by calculating complex scattering phase shifts.[34] Details of this scattering model are already discussed in our recent papers on different atomic and molecular targets[22−27] and hence are not given here.

Now the total inelastic cross section $Q_{\rm inel}$ includes all possible ionization as well as excitation processes, and hence we have

$$Q_{\rm inel}(E_{\rm i}) = \Sigma Q_{\rm ion}(E_{\rm i}) + \Sigma Q_{\rm exc}(E_{\rm i}), \quad (5)$$

where the first term corresponds to the total cross sections for all allowed ionizations of the target by electron impact, and the second term includes cumulatively all possible electronic transitions dominated by low-lying states, for which the threshold values lie below the first ionization energy I.[35] In this paper, our interest focuses on the cumulative inelastic processes induced by incident electrons.

Now, the microscopic cross section $Q_{\rm inel}$ can be incorporated as an input for the calculation of macroscopic quantity IMFP. First, we define the macroscopic cross section Σ[36] as the mean number of specific kind of collisions of electrons per unit length in a material having N target atoms/molecules per cm^3. Thus

$$\Sigma = NQ, \quad (6)$$

where Q is the microscopic cross section, which is $Q_{\rm inel}$ in our case. Moreover,

$$N = \frac{\rho N_{\rm A}}{M}, \quad (7)$$

where ρ is the Bulk density in gm/cm^3, $N_{\rm A}$ is the Avogadro number (6.02×10^{23} molecules per mole), and M is the Molar mass in gm/mol. Thus, in the case of inelastic scattering, the macroscopic cross section is expressed by

$$\Sigma_{\rm inel} = NQ_{\rm inel}. \quad (8)$$

This quantity (expressed in length^{-1}) can be used to estimate the energy lost by incident electron per unit path length in a medium. Finally, the mean free path for inelastic scattering $\lambda_{\rm inel}$ is defined as

$$\lambda_{\rm inel} = \frac{1}{\Sigma_{\rm inel}}. \quad (9)$$

3. Results and discussion

The aim of the present work is to carry out approximate calculations of IMFP for the present targets, and this is meaningful since the minimum IMFP reported previously has shown large variations. In the present theoretical model of electron scattering, we first calculate the total inelastic cross section $Q_{\rm inel}$ for electron–atom/molecule collisions using the complex potential, as discussed in Section 2. The present complex potential includes the effect of bulk medium through the target charge density as given by Salvat *et al.*[31] The methodology in Section 2 is employed to calculate the IMFP for Si, SiO_2, and Al_2O_3 in their

crystalline forms, while SiO has only been considered in the amorphous state. Some details of solid SiO are discussed in Ref. [37].

To determine theoretically the IMFP of electrons in a medium, our first task is to calculate the single scattering atomic/molecular inelastic cross section $Q_{\rm inel}$ at different incident energies. We have shown calculated results for Si atoms bound in solid (metal) in Fig. 1, which are compared with that of the free Si atoms. The absorption potential for free or isolated silicon atom is calculated based on the free-atom charge density at the corresponding ionization energy, i.e., 8.15 eV. The free-atom cross sections are in a good accord with the available data in one of our earlier papers,[26] which verified the correctness of the present method. As can be seen from Fig. 1, the $Q_{\rm inel}$ of the free Si atoms is much larger than that of the solid (metal) Si atoms in the energy below 100 eV. These two cross section results tend to merge at higher energies beyond 300 eV. The difference between the results for free and bound atoms is reasonable and can be attributed to the differences in the charge density and the inelastic threshold. The maximum $Q_{\rm inel}$ obtained with the microscopic (i.e., quantum mechanical) approach corresponds to the minimum in the IMFP for the respective bulk material.

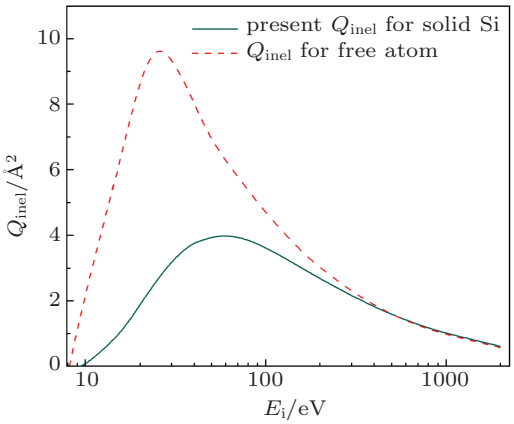


Fig. 1. (colour online) Present total inelastic cross sections $Q_{\rm inel}$ for electron impact on Si atom in two phases.

With these sample results of $Q_{\rm inel}$ (see Fig. 1) for one of our target systems Si, let us now calculate the IMFP. The required bulk physical properties of different target materials given in Table 1 are utilized in Eqs. (7)–(9).

Table 1. Bulk properties of the target materials used in the present work. All solids mentioned are crystalline except SiO which is amorphous.

Solid	$I_{\rm p}$/eV	$E_{\rm g}$/eV	ρ/g·cm^{-3}	M/g·mol^{-1}	R/Å
Si	8.15	1.11	2.33	28.08	Si–Si=2.35
SiO_2	12.13	8.90	2.19	60.08	Si–O=1.62, O–O= 2.62
SiO	11.49	–	2.13	44.08	Si–O=1.48
Al_2O_3	8.9	8.28	3.95	101.96	Al–O=1.80

In Fig. 2, the present results for the IMFP of electrons in bulk silicon are shown along with the relevant experimental and theoretical data available from several other studies.

We have included in Fig. 2, a single data point at a low energy of 11 eV, adopted from the universal IMFP data curve.[38,39] The reason to call it universal curve is that it is an approximate common curve showing $\lambda_{\rm IMFP}$ of all the metallic elements. Inelastic scattering of electrons in the energy range of 10–2000 eV mostly involves excitations of conduction electrons, which have more or less the same number density in all metallic elements. The universal curve in Refs. [38] and [39] exhibits a broad minimum in IMFP around 70 eV. Our present results on Si also show a dip of $\lambda_{\rm IMFP}$ = 5.02 Å around 65 eV. Towards lower energies we have extrapolated smoothly and merged the present $\lambda_{\rm IMFP}$ values with the single data point as shown in Fig. 2, although we note that this is an approximate procedure. The minimum value of $\lambda_{\rm IMFP}$ corresponds to the most intense inelastic interactions of incident electrons in the Si in bulk. Note that at lower energies other mechanisms like the scattering with phonons will be important, but not included presently.

Overall good agreement can be achieved for the present results with Tanuma *et al.*[17] at low-energy (below 200 eV) region, and with Koch *et al.*[7] and Tung *et al.*[4] in the high-energy (> 200 eV) region (see Fig. 2). However, a point worth of noting here is that there are marked discrepancies in the available data. From optical data of Tung *et al.*,[4] the lowest

available (but not the minimum) $\lambda_{\rm IMFP}$ is 1.38 Å for electrons with an energy of 40 eV. The lowest value predicted by Tanuma *et al.*[17] is 4.07 Å for electrons with an energy of 50 eV, which is in close agreement with Gries *et al.*[3] Experimental data of Lesiak *et al.*[6] and Gergely *et al.*[5] are in close mutual agreement (see Fig. 2).

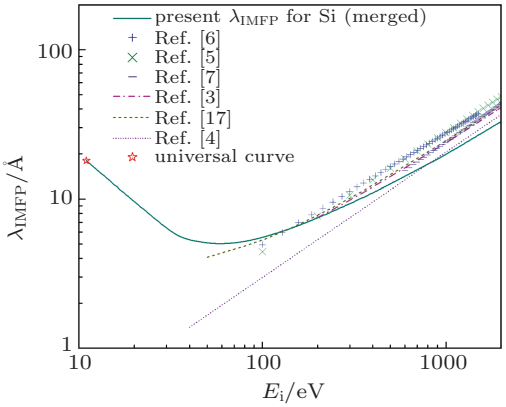


Fig. 2. (colour online) Inelastic mean free path $\lambda_{\rm IMFP}$ of electrons in Silicon.

Next, figure 3 shows the IMFP results for SiO_2 with parameter $\Delta = 21.03$ eV in Eq. (2). Theoretical work of Tanuma *et al.*,[18] Akkerman *et al.*,[40] Chen *et al.*,[41] as well as Ashley and Anderson[42] on IMFP determination is based on the optical data along with their theoretical model. Here we have compared our $\lambda_{\rm IMFP}$ results of SiO_2 with the available theoretical data since no experimental results are available for the electron IMFP in SiO_2. As in the case of Si, a large difference is also observed for the minimum IMFP. Present results are in good agreement with Tanuma *et al.*[18] and Chen *et al.*[41] Various other results available do not point to a minimum of $\lambda_{\rm IMFP}$ as a function of energy. The present results show the minimum value of 7.55 Å at about 100 eV. In order to extend the present results down to the minimum $\lambda_{\rm IMFP}$, we have averaged out the available IMFP data below 100 eV and extrapolated our values to this average value down to 50 eV.

An attempt is also made to calculate the IMFP for SiO in amorphous form. Figure 4 shows the present calculation results of IMFP for SiO with the threshold energy parameter $\Delta = 11.49$ eV in the electron energy range from 20 eV to 2 keV. Since there is a lack of experimental or theoretical data for this target, we have compared the present results with the present $\lambda_{\rm IMFP}$ for Si and SiO_2, as depicted in Fig. 4. Compared with crystalline Si and SiO_2, the amorphous form of SiO offers the IMFP calculation for electron energies down to 20 eV.

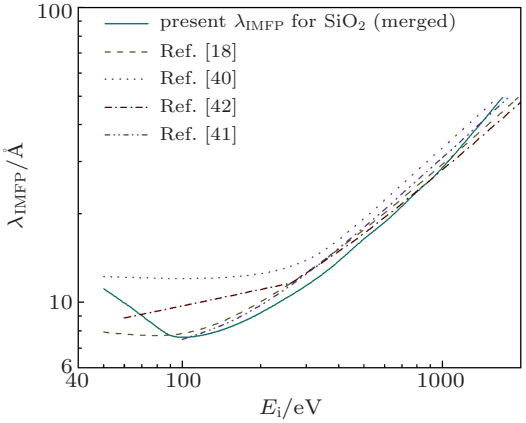


Fig. 3. (colour online) Inelastic mean free path $\lambda_{\rm IMFP}$ of electrons in SiO_2.

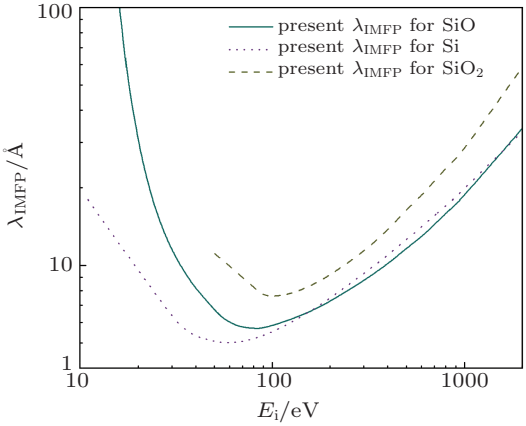


Fig. 4. (colour online) Inelastic mean free path $\lambda_{\rm IMFP}$ of electrons.

Finally, the IMFP for Al_2O_3 in its crystalline form (with $\Delta = 17.2$ eV) is presented in Fig. 5. Comparison is made with the data of Tanuma *et al.*,[17] Akkerman

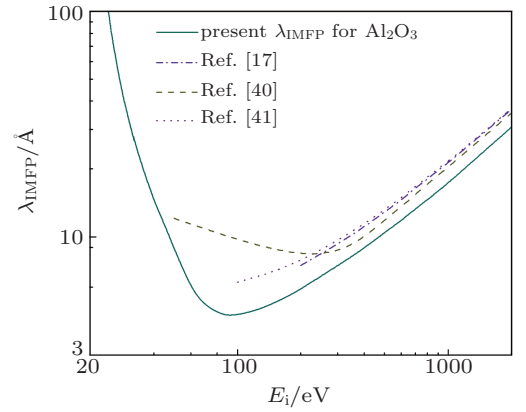


Fig. 5. (colour online) Inelastic mean free path $\lambda_{\rm IMFP}$ of electrons in Al_2O_3.

et al.,[40] and Chen *et al.*[41] There is a marked deviation between the IMFP data of Akkerman,[40] Tanuma *et al.*,[17] and Chen *et al.*[41] The only well defined minima for IMFP of 7.2 Å is observed in Ref. [40] at higher value of electron energy. The present results fall slightly below the available IMFP data with the minimum value of 4.49 Å for electrons at 90 eV. Below 200 eV there is a marked deviation among the available IMFP data for Al_2O_3 (see Fig. 5).

Finally, the minimum IMFP found for different target materials along with the corresponding incident energy is exhibited in Table 2.

Table 2. Minimum IMFP values for present target as a function of incident electron energy.

Target in bulk	Minimum IMFP/Å	Electron energy/eV
Si	5.02	65
SiO	5.70	81
SiO_2	7.55	100
Al_2O_3	4.49	90

4. Conclusions

Marked discrepancy in the available IMFP data for Si, SiO_2, and Al_2O_3 has prompted us to choose these targets for the present calculations. Also chosen in this work is an amorphous target SiO for which there is almost no previous work on electron IMFP. Presently we have successfully implemented our semi-empirical quantum mechanical approach which starts with electron–atom/molecule inelastic scattering. Inelastic scattering cross sections extracted theoretically are used to obtain λ_{IMFP} for the present targets, and an attempt is also made to predict the minimum IMFP in each case. Let us emphasize that the results on IMFP reported in literatures either do not show a minimum or exhibit a dip differing in position as well as magnitude for the same target. Therefore, the present calculations are of interest and relevance, although they are approximate. Particularly in the case of amorphous targets, the approach is promising since the constraints of crystalline structure are relaxed in such cases.

Potential applications of the present theoretical work are quite general. These include electron impact studies with solid matter existing in outer-space environments. For objects in planetary and solar systems together with moon and other satellites having almost no atmosphere, charged particles like electrons are expected to reach and interact with the solid terrain. Therefore, the calculation of IMFP, as we just discussed, can be a meaningful study.

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