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Elastic scattering of electrons by silicon, germanium and tin tetrahalides

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ABSTRACT

This article reports the elastic collision cross section for the tetrahedral compounds of silicon, germanium and tin by intermediate to high energy (20–5000 eV) electrons. The calculations were carried out using a quantum mechanical approach called spherical complex optical potential (SCOP) formalism. Under the same frame work the total scattering cross section has been also studied. Among the studied molecules, the total scattering cross sections for $SiCl_4$ and $GeCl_4$ by electrons has been compared with available experimental values. For all other molecules the elastic and total cross sections are reported for the first time. We have also investigated the halogenation effect by comparing the ratio of cross sections for different halides.

1. Introduction

Electron induced elastic and inelastic cross sections are important for modeling and controlling discharge environments in low-temperature plasma reactors. The present interest in cross section data for silicon and germanium tetrahedral compounds is primarily due to their importance in low temperature plasmas, microelectronic industry and several other industrial plasmas. In our previous work, we reported total inelastic and ionization cross sections for the present molecules [1]. All these molecules are in tetrahedral geometry with T_d point group. Because of their simple geometrical structure and near spherical arrangements of atoms, theoretical approximations are appropriate and well justified to be employed for the calculation of cross sections. In view of this, there are some previous efforts to report data for some of these molecules. The elastic cross sections of all tetrahalides except tin were calculated by Możejko et al. [2] employing independent atom method with static-polarization model potential. Szmytkowski et al. [3] measured absolute total scattering cross section for $GeCl_4$ molecule from 0.6 to 250 eV energy. The absolute total cross sections for e-$SiCl_4$ system have been measured by Możejko et al. [4] in two distinct electron-transmission experiments, in Gdańsk and in Trento laboratory, for impact energies ranging from 0.3 to 250 eV and from 75 to 4000 eV, respectively. Besides these, there are no other reported data on these molecules to the best of our knowledge. Hence, it is quite evident from literature survey that cross section data for these molecules are scarce and fragmentary. Therefore, we have taken this task to calculate electron impact total cross section using spherical complex optical potential (SCOP) method [5,6] in the energy range 20–5000 eV. It is hoped that this work would be beneficial to understand physical and chemical processes of low-temperature plasmas in many fields of applied interest.

2. Theoretical method

For the calculation of cross sections by electron impact on the target molecules, we have adopted the SCOP method [5,6], a quantum mechanical approach having realistic accuracy. As the molecules of present interests are quite large, considering them as single scattering centre would be unreasonable. To simplify the methodology, the constituent atoms are assumed to be independent scattering centres to the incoming electrons. This approximation is justified since, at intermediate to high energies, electron is assumed to interact with individual atoms on its path depending on the position and angle of scattering. However, to include the molecular nature of the targets, we have used the molecular properties of respective targets while computing the cross sections. The target properties considered here are its structure (through bond length and charge density), molecular ionization threshold and dielectric polarizability. This method of evaluating cross section for the molecular target is called the

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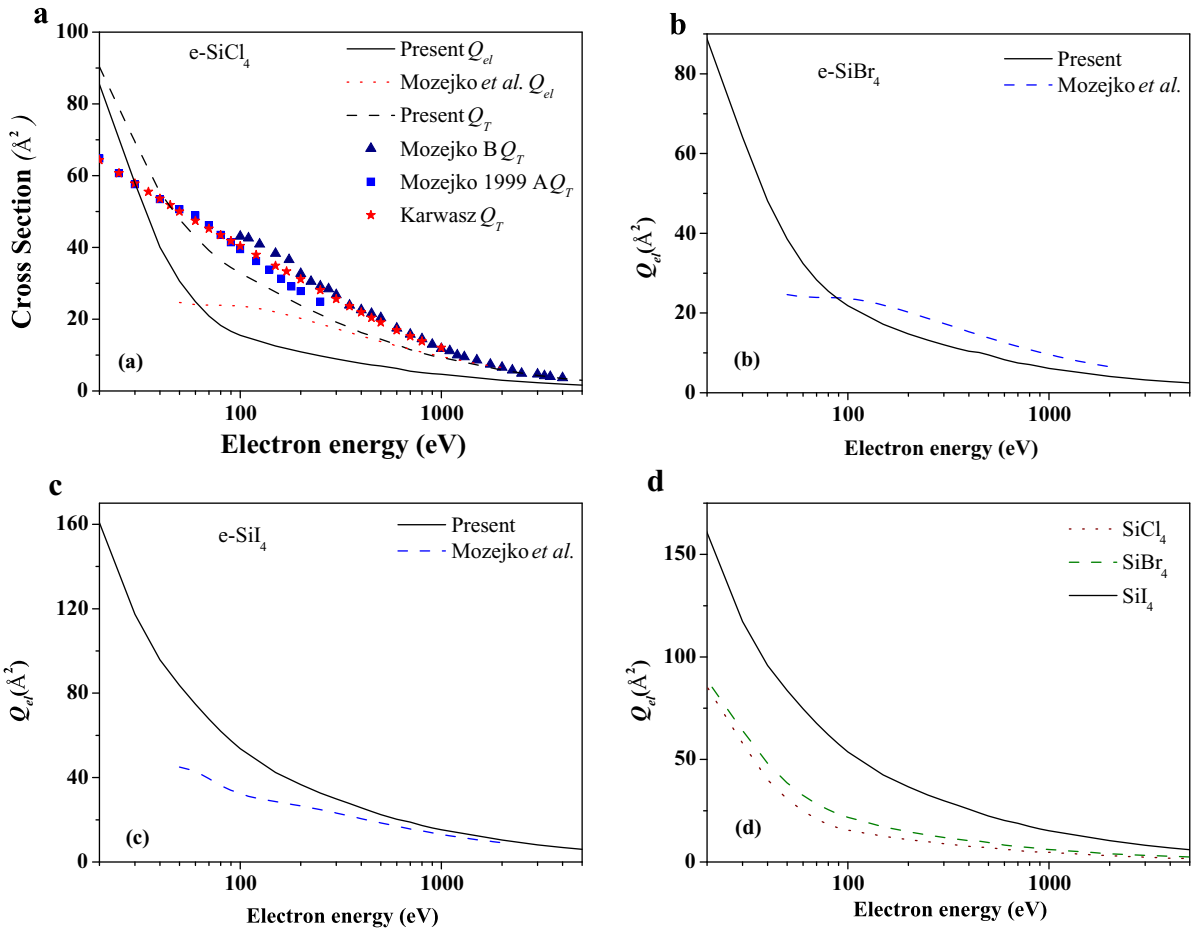

Fig. 1. (a) Q_{el} and Q_T e-$SiCl_4$. Solid line: Present Q_{el}; short dash line: Mozejko et al. [2], dash line: Present Q_T; triangles: Możejko et al. [4]; squares: Możejko et al. [4]; stars: Karwasz [15]. (b) and (c) Q_{el} for e-$SiBr_4$ and e-SiI_4. Solid line: Present; dash line: Możejko et al. [2] and Figure (d) Influence of the peripheral atoms in the Q_{el}. Solid line: $SiCl_4$; dash line: $SiBr_4$ and dotted line: SiI_4.

modified additivity rule (MAR). The elastic cross sections (Q_{el}) for each scattering centre is calculated independently using the SCOP method [5,6]. Then by adding individual cross section of each centres we get the total elastic cross section. Here, the interaction between the projectile electron and the target molecule is established through a spherical complex optical potential [7]. Employing this potential in the Schrödinger equation to solve it using the partial wave analysis method, we obtain complex phase shifts as output. These phase shifts are used to compute various cross sections. The interaction potential of the e-target scattering system is represented by,

$$V_{opt}(r, E_i) = V_R(r, E_i) + iV_I(r, E_i) \quad (1)$$

Here, the real part of the potential is given by:

$$V_R(r, E_i) = V_{st}(r) + V_{ex}(r, E_i) + V_p(r, E_i) \quad (2)$$

r is the radial distance between the incident electron and the target and E_i is the incident electron energy. The first term of Eq. (1) represents the electron target interaction through various real potentials of the system namely, static, exchange and polarization potentials. The non-spherical terms due to vibrational and rotational excitation of the target are not considered in this approach. The Cox and Bonham [8] Hartree-Fock parameters are used to derive static potential (V_{st}). The parameter free Hara's [9] free electron gas exchange model is used here to formulate exchange potential (V_{ex}) and Zhang et al. [10] model is employed for the polarization-correlation potential (V_p). The absorption potential, which forms the imaginary part of Eq. (1), is given by [11],

$$V_{abs}(r, E_i) = -\rho(r)\sqrt{\frac{T_{loc}}{2}}\left(\frac{8\pi}{10k_F^3 E_i}\right)\cdot\theta\left(p^2 - k_F^2 - 2\Delta\right)\cdot(A_1 + A_2 + A_3) \quad (3)$$

Where, $T_{loc} = E_i - (V_{st} + V_{ex} + V_{Pol})$ is the local kinetic energy of the projectile electron, p is the linear momentum, determined from $p^2 = 2E_i$, $k_f = \sqrt[3]{3\pi^2\rho(r)}$ is the Fermi wave vector and A_1, A_2 and A_3 are dynamic functions depending on Heaviside unit step-function $\theta(x)$, ionization potential (IP) and Δ. Δ is an energy dependent parameter, which determines a threshold below which $V_{abs} = 0$. However, Δ is fixed to a minimum value of IP in the present case, in cognizant with the original work of Staszewska et al. [11], as the energy of interest is above the ionization threshold of the targets. In this way, the full complex potential for a given electron-scattering centre system is constructed. For the construction of these potentials the target properties such as ionization potential (IP) and polarizability of the target molecule are used, which are listed in Table 1. After having the potential, the Schrödinger equation is solved numerically by Numerov method using partial wave analysis. Initially only few partial waves are required at low incident energies, which increases gradually as the incident energy increases and more and more partial waves will be required for convergence. These phase shifts carry the signature of various electron-molecule scattering phenomena. Hence they are

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