J. At. Mol. Sci.
doi: 10.4208/jams.022812.032212a

Vol. **4** , No. 1 , pp. 41-48
February 2013

Electron-impact ionization of SiCl, $SiCl_2$ and $SiCl_4$ molecules

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Received 28 February 2012; Accepted (in revised version) 22 March 2012
Published Online 8 December 2012

Abstract. Total ionization collision cross sections are calculated for silicon chloride compounds namely SiCl, $SiCl_2$ and $SiCl_4$ applying binary -encounter - Bethe (BEB) and modified BEB model for projectile energy from the ionization threshold to 1000 eV. The total ionization cross sections obtained using the binary-encounter-Bethe (BEB) model and the modified BEB model are compared with experimental and theoretical results. This model has been found to be successful for a wide range of molecules but for silicon chloride molecules the results are not in good agreement with experimental data.

PACS: 34.80.Gs, 52.20.Fs

Key words: electron impact ionization, ionization cross sections, BEB model

1 Introduction

The ionization of an atom or molecule by electron impact is one of the most fundamental electron collision processes. The study of electron impact ionization of molecule play a key role in many applications such as radiation and environmental chemistry, gas discharges and gas lasers, fusion edge plasmas and plasma processing of materials [1-3], light-stimulated chemical vapor deposition in the microelectronic industry [4].

Nanocrystalline silicon and polycrystalline silicon films have successful applications in various optoelectronic devices, such as thin film solar cells, thin film transistors, switching devices and so on [5,6]. For depositing poly Silicon films, $SiCl_4/H_2$ mixture gas is used by plasma enhanced chemical vapor deposition. $SiCl_4$ is also used as an admixture in processing plasma feed gas mixtures which are used for selective reactive ion etching of GaAs on AlGaAs [7] and for characterization of polyester fabrics treated in $SiCl_4$ plasma [8,9]. In all these applications, electron impact ionization cross sections with SiCl,

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$SiCl_2$ and $SiCl_4$ are very important quantities for the understanding and modeling of the interaction of silicon -chlorine plasmas with materials.

Mahony *et al.* [10] have measured total ionization cross sections for SiCl and $SiCl_2$ from threshold to 200 eV using the fast-neutral-beam technique. Becker *et al.* [11] have measured electron impact ionization of $SiCl_x$ (x=1-4) using a time-of-flight mass spectrometer (TOF-MS) and a fast-neutral-beam techniques. The energy range covered in the TOF-MS was from the ionization threshold to 900 eV and up to 200 eV in fast-neutral-beam apparatus. Basner *et al.* [12] have measured electron impact ionization of $SiCl_4$ using two different experimental techniques namely, a time-of-flight mass spectrometer (TOF-MS) and a fast-neutral-beam techniques. The energy range covered in the TOF-MS was from the ionization threshold to 900 eV and up to 200 eV in fast-neutral-beam apparatus. The absolute total cross-sections for electron scattering on $SiCl_4$ molecules have been measured by Mozejko *et al.* [13] in two distinct electron-transmission experiments, in Gdansk and in Trento laboratory, for impact energy ranging from 0.3 to 250 eV and from 75 to 4000 eV, respectively. Recently, King and Price [14] have measured relative partial ionization cross sections (PICS) for the formation of fragment ions following electron ionization of $SiCl_4$, in the electron energy range 30-200 eV, using timeof-flight mass spectrometry coupled with an ion coincidence technique.

From theoretical side, the authors [10-12] have calculated the total ionization cross sections using DM formalism. Deutsch *et al.* [15] have calculated the ionization cross sections of $SiCl_x$ (x=1-4) using a modified additivity rule (MAR) in the energy range from 30 to 200 eV. Recently Kothari *et al.* [16] have reported the ionization cross sections of $SiCl_x$ (x=1-4) using their complex scattering potential - ionization contribution (CSP-ic) method.

The binary-encounter-Bethe (BEB) model of Kim and Rudd [17] has produced total ionization cross -sections in good agreement with experimental data for many important gases. It has become a useful tool for supplying cross-section data and also for identifying reliable sets of experimental data. Hwang *et al.* [18] have found that the BEB model was underestimating the cross-section by a significant margin for heavy atoms with the highest principal quantum number $n' \geq 3$, or molecules containing heavy atoms. In order to bring the BEB cross sections into satisfactory accord with experiment, they introduced a scaling factor $1/n_i$ into the expression for the BEB cross-section whenever $n_i' \geq 3$. Here n_i being the principal quantum number of orbital i. For molecules, this scaling was introduced whenever the Muliken population analysis showed that the orbitals were dominated by the high n orbital of the heavy atom. In this article, the total ionization cross sections for SiCl, $SiCl_2$ and $SiCl_4$ molecules are obtained using both, the BEB model and the modified BEB model.