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K-shell ionization cross sections of light atoms due to electron impact

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Abstract. Electron impact ionization cross sections (EIICS) of K-shell have been evaluated for light atoms (C, N, O) at incident energies ranging from ionization threshold to 1 GeV. The plane wave Born approximation is used in the proposed model by incorporating it in exchange, coulomb and relativistic effects along with the contributions of transverse interaction to ionization cross sections. In present model, we require two constants for each atom, ionization energy (I) and the electron occupation number (N). Adequate comparisons have been made with other theoretical methods, empirical formulae. The predicted EIICS of K-shell also compared with experimental data. Obtained results are in good agreements with available experimental data.

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Key words: ionization cross section, electron impact, K-shell

1 Introduction

In recent years there has been an upsurge of interest in the evolution of the theoretical cross sections of atoms and molecules due to photons, electron and heavy particle impact because of their usefulness in many fields. For example cross sections for K-shell ionization are needed for modeling of radiation effects in materials, in biomedical research and modeling of fusion plasma in tokomaks. There is also a strong impact on many other scientific areas. Among those are astrophysics and astrochemistry, atmospheric physics, radiobiology and radiation chemistry, x-ray laser and fusion research. Electron impact ionization cross sections (EIICS) at high energy have great importance in many accelerator applications. The computed data on cross sections are necessary in studying the problems of radiative association. Carbon (C), nitrogen (N) and oxygen (O) have great importance in the study of astronomy, radiobiological effects, due to Auger electrons [1–3].

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For K-shell ionization of atom by electron impact, the cross sections have been obtained both theoretically and experimentally by various groups since 1940s. First of all classical formula for K-shell theory is given by Gryzinski [4], which provides a fairly good description over a wide energy range except near the threshold region which was further modified by Deutsch and Mark [5] for atomic ionization cross sections. Later on, quantum mechanically the theory based on first order perturbation and Hartree-Slater-Fock wave function put forward [6]. Next step was the plane wave Born approximation (PWBA) [7] and distorted wave Born approximation (DWBA) [8,9] came into light. Several researchers [10–14] have proposed many empirical and semi empirical models expressions for K-shell ionization cross section to fit the experimental data. None of them has been successful completely to describe experimental cross sections data over a wide range of incident electron energies.

Casnati *et al.* [11] proffered an empirical model to describe cross sections for $6<Z<79$. Bell *et al.* [13] proposed their analytical formulae for EIICS referred as BELL involving species-dependent parameters for the determination. Bell et al. used analytical formula for ions and light atoms with $Z\leq 8$ but BELL formula lacks in relativistic component. Talukder *et al.* [15] proposed SBELL model, taking into account relativistic and ionic effects. Empirical model by Hombourger [12] provide a good fits to the K- shell data. In 2003 Santos *et al.* [16] have given the relativistic version of the BEB model to calculate the cross sections for K-shell ionization of atoms that requires two constants, the binding energy and average kinetic energy of K electrons.

In 1995, Khare and Wadehra [17] have calculated the EIICS for K-shell for a numbers of atoms. They have employed the plane wave Born approximation (PWBA) with corrections for exchange, coulomb and relativistic effects. For the positron and electron impact, Khare and Wadehra [7] have calculated the acceleration and deceleration energy of the coulomb field of the bare nucleus for the hydrogen like atom. They have shown the coulomb energy $E_c=hI/[1+F(x)]$, where $h=4n^2/[3n^2-l(l+1)]$, n and l are the principal quantum number and angular quantum number respectively. $F(x)$ is the function of the $x=2Zr_-/a_0$, Z and a_0 are the atomic number and Bohr radius. r_- is the shortest distance from the centre of the atom at which electron or positron reaches in the collision process. They have taken $r_-=0$, so $F(x)=0$ for the electron and hence consider the upper limit with the relativistic correction only.

In this paper we have consider the relativistic correction in the upper limit as well as in the lower limit of the integration to calculate the EIICS. In case of lower limit instead of taking $F(x)=0$ [7], we put forward to assign a finite value to $F(x)$, which was obtained by fitting it on reliable measured EIICS for light atom. Present model prevail a high degree of goodness of cross sections to the experimental data.

2 Theory

In 1999, Khare *et al.* [18] proposed a model to calculate the EIICS for molecules by combining the useful features of two models of Kim *et al.* [19] and Saksena *et al.* [20], where they replaced $(1-\omega/E)$ by $(E'/E'+U+I)$, where ω is the energy lose suffered by incident electron