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K-shell ionization cross sections of transition and non metals by electron impacts

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Abstract. The theoretical model, developed by Khare, has been modified to calculate the total cross sections for K-shell ionization of 12 atom targets (C, N, O, Al, Fe, Se, Ag, Sb, Ho, Au, Bi, U) due to electron impact at incident electron energy from ionization threshold to 1 GeV. The various calculated cross sections are in remarkable agreement with available experimental data and other theoretical cross sections.

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

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1 Introduction

Electron impact ionization cross sections for K-shell ionization are needed for modeling of radiation effects in materials, in biomedical research and modeling of fusion plasmas in tokomaks. The electron impact ionization cross sections find important applications in fields such as mass spectrometry, radiation science, semiconductor physics, atmosphere physics, astrophysics, x-ray laser and fusion research. The computed data on cross sections are necessary in studying the problems of radiative association. Over the past five decades, many experimental and theoretical studies have been carried out to estimate the electron impact K-shell ionization cross section by various groups.

In this paper, we have modified the Khare *et al.* [1] model for K-shell ionization. First of all, the classical formula for K-shell ionization is given by Gryzinski [2], which provides a fairly good description over a wide energy range except near the threshold region. This formula was further modified by Deutsch *et al.* [3] for atomic ionization cross sections covering the whole energy range. Their formula uses weighted sum of the squared radii of the maximum charge

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density of the electron subshells. The final expression involves a number of parameters which are different for *s*, *p* and *d* bound electrons and are different from those given by Gryzinski. An additional relativistic factor was also introduced empirically by the above authors to fit the theoretical cross sections with experimental data. Later on, quantum mechanically the theory based on the Plane Wave Born Approximation (PWBA) [4–6] and Distorted Wave Born Approximation (DWBA) [7] came into light.

In ultrarelativstic energy region, Scofield [7] employed the first Born approximation (FBA), in which he represented incident and scattered electrons by plane waves, obtained by solving the free particle Dirac equation and the active electron of each target, moving in a central field, was also treated relativistically. His cross sections exhibit a nice agreement with the experimental data at ultrarelativstic energies. However, these methods fail at impact energies near threshold of ionization. Hombourger [8] calculated the K shell ionization cross sections by proposing a relativistic empirical expression through an analysis of experimental data for atoms ($6 \leq Z \leq 76$). For the electron impact ionization cross sections, Bell *et al.* [9] have developed analytical formulae, referred as BELL formulae, involving species-dependent parameters. Casnati *et al.* [10] proposed another empirical model to describe cross sections for ($6 < Z < 79$).

Khare *et al.* [4–6] have calculated the electron impact ionization cross sections for K-shell for a numbers of atoms. They have employed the PWBA with corrections for exchange, coulomb and relativistic effects. In 2000 Kim *et al.* [11] proposed the relativistic version of the BEB model [12]. Kim *et al.* [11] and Santos *et al.* [13] calculated the cross sections for K-shell ionization of atoms by using their relativistic BEB formula.Recently many researchers like Haque *et al.* [14], Uddin *et al.* [15], Patoatry *et al.* [16], Huo [17], Talukder *et al.* [18] etc. have calculated the K shell ionization cross sections by modifying the different model from threshold to ultrarelativistic energy range.

In 1999 Khare *et al.* [1] proposed a model, referred as Khare [BEB] model, to calculate the ionization cross sections for molecules This model has been developed by combining the useful features of PWBA [19] and BEB model of Kim and Rudd [12], where $(1-\omega/E)$ was replaced by (E_r/E_r+I+U), ω is the energy lose suffered by incident electron in the ionizing collision, E_r is the relativistic kinetic energy of incident electron, I is the ionization energy, U is the average kinetic energy of bound electron. Here $I+U$ represent the increase in kinetic energy of the incident electron due to its acceleration by the field of the target nucleus. Furthermore, they have employed the useful features of the Binary Encounter Bethe models of Kim and Rudd [12]. Kim and Rudd [12] have used the COOS $df/d\omega = NI/\omega^2$ and dropped the contribution of exchange to Bethe term. Although Bethe and Mott cross-sections in Khare *et al.* [1] model are different corresponding cross-sections of Kim [BEB] model but the total ionization cross sections obtained in both model are very close to each other.

For the positron and electron impact Khare *et al.* [5] have calculated the deacceleration and acceleration energy of the coulomb field of the bare nucleus for the hydrogen like atom. They have shown that 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