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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 in the ionizing collision, E is the kinetic energy of incident electron, E' is the relativistic energy, I is the ionization energy, U is the average kinetic energy of bound electron. Here $U+I$ represent the increase in kinetic energy of the incident electron due to its acceleration by the field of the target nucleus.

Presently we have replaced $(U+I)$ of the Khare model by $hI/[1+F(x)]$, with relativistic effect, attraction by target nucleus, for K- shell ionization. In present model to calculate the K-shell ionization cross sections require two constants for each atom, ionization energy (I) and the occupation number (N). For fully occupied K-shell N will be 2. The total electron impact ionization cross section is given by

$$\sigma_T = \sigma_{PBB} + \sigma_{PMB} + \sigma_t, \tag{1}$$

where σ_{PBB}, σ_{PMB} and σ_t are the Bethe's, Mott's cross section and the cross section due to transverse interaction respectively.

Bethe cross section section is expressed as

$$\sigma_{PBB} = \frac{SI_r^2}{(t+f)} \int_{I_r}^{E_r} \frac{1}{\omega^3} \ln\left(\frac{\omega}{Q_-}\right) d\omega. \tag{2}$$

The recoil energy Q_- is given by [18]

$$Q_- = 0.5mc^2 \left(\left(E_r(E_r-\omega)\right)^{1/2} - \left((E_r-\omega)(E_r-\omega+2mc^2)\right)^{1/2} \right)^2. \tag{3}$$

It is due to the assumption that a large contribution to the integral comes from the small values of ω. Hence for $\omega \ll E_r$, we obtain from Eq. (3)

$$Q_- = \frac{\omega^2}{4} \left(\frac{1}{2} mc^2 + \frac{1}{E_r} \right). \tag{4}$$

Now putting this into the Eq. (2) and evaluating the integral we obtain

$$\sigma_{PBB} = \left(\frac{S}{t+f}\right) \left(0.4431 \left(1 - \frac{1}{t^2}\right) - 0.5 \ln\left(\frac{1}{t} + \frac{I_r}{2mc^2}\right) + \frac{1}{2t^2} \ln\left(1 + \frac{E_r}{2mc^2}\right) \right). \tag{5}$$

Mott cross section is

$$\sigma_{PMB} = \left(\frac{S}{t+f}\right) \left(\left(1 - \frac{2}{t+1} + \frac{t-1}{2t^2}\right) + \left(\frac{5-t^2}{2(t+1)^2} - \frac{1}{t(t+1)}\right) - \left(\frac{(t+1)}{t^2} \ln\left(\frac{t+1}{2}\right)\right) \right) \tag{6}$$

and the cross section due to transverse interaction is

$$\sigma_t = -\frac{SI_r^2}{NR(t+f)} M^2 \left(\ln(1-\beta^2) + \beta^2 \right) \tag{7}$$

with $S=AN/I_r^2$, $t=E_r/I_r$, the relativistic energy E_r is

$$E_r=\frac{1}{2}mv^2=\frac{1}{2}mc^2\left(1-\frac{1}{\left(1+\frac{E}{mc^2}\right)^2}\right), \tag{8}$$

$$I_r=\frac{1}{2}mv_b^2=\frac{1}{2}mc^2\left(1-\frac{1}{\left(1+\frac{I}{mc^2}\right)^2}\right), \tag{9}$$

$$f=\left(\frac{h}{1+F}\right). \tag{10}$$

In Eq. (10), we have proposed the value of F by

$$F=\zeta Z, \tag{11}$$

$\zeta=0.011$ and $h=1.67$ for k shell ionization. The Bethe collision parameter is given by

$$b_{nl}=\frac{I_r M^2}{Z_{nl}R}, \tag{12}$$

where Z_{nl} is the number of electrons in the (nl) sub-shell of the atom. With $N=Z_{nl}$ and from Eq. (12), Eq. (7) becomes

$$\sigma_t=-\frac{S b_{nl}}{(t+f)}\left(\ln(1-\beta^2)+\beta^2\right), \tag{13}$$

the value of b_{nl} in the Khare parameter [21] is given by

$$b_{nl}=\alpha p^{-\gamma}, \tag{14}$$

where $p=I/I_s$, $I_s=Z_s^2R$, and the value of α and γ for K-shell is $\alpha=0.285$ and $\gamma=1.70$.

In this paper, we denote these quantities as follows:

$A=4\pi a_0^2R^2$,	$R=$Rydberg energy;
$a_0=$first Bohr radiu,	$N=$number of electrons;
$I=$ionization thresholds,	$m=$rest mass of electron;
$E_r=$relativistic energy,	$v=$incident velocity;
$c=$velocity of light,	$Q_-=$recoil energy;
$\omega=$the energy loss,	$Z_s=$the effective atomic number;

$M^2=$total dipole matrix squared for the ionization;
$v_b=$the speed of an electron with the kinetic energy$I$;
$\beta=$the ratio of the incident velocity and the velocity of light.

3 Results and discussion

In this paper, we present our results for electron impact ionization cross sections as a function of electron impact energy. EIICS have been calculated for the three light atoms (C, N, O) by the modified formula. From Eq. (1) the ionization cross sections σ_T have been calculated for K-shell of each atom for incident energy E varying from threshold ionization energy to high energy (1 GeV). Predicted EIICS is the sum of Eqs. (5), (6) and (13). To access the level of performance of the present model, its predictions are compared with the result from the available other theoretical and experimental data. Present results are in good to excellent agreement with available experimental data.

In Fig. 1, we have plotted electron impact ionization cross sections (EIICS) versus E from threshold to 1 GeV for carbon atom. Obtained results compared along with the experimental data given by Tawara *et al.* [22], Isaacson [23], Hink and Paschke [24], Egerton [25] and theoretical data set of Casnati *et al.* [11], Hombourger [12], and Kim and Desclaux [26]. Present cross sections are in good accordance with the experimental data of Tawara *et al.* [22], Isaacson [23], Hink and Paschke [24], and Egerton [25]. Other theoretical cross sections by Kim and Desclaux [26] is in excellent agreement with obtained results.The difference between predicted results and the data by Hombourger [12] and Casnati *et al.* [11] are more at low energies while at high energies present results merge with them.

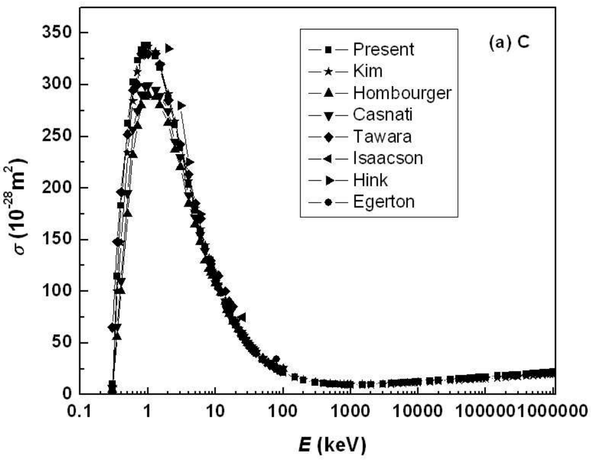

Figure 1: Comparison between the present theoretical EIICS and the experimental EIICS for carbon (C). ■, present work; ★, theoretical data by Kim and Desclaux [26]; ▲, theoretical data by Hombourger [12]; ▼, theoretical data by Casnati *et al.* [11]; ♦, experimental data by Tawarai *et al.* [22]; ◄, experimental data by Isaacson [23]; ►, experimental data by Hink and Paschke [24]; •, experimental data by Egerton [25].

Fig. 2 shows the ionization cross section for nitrogen atom for K-shell. We have compared the data of nitrogen. There are three experimental data, named Tawara *et al.* [22], Glupe and Mehlhorn [27], and Isaacson [23]. Previously theoretical data are reported by Kim and Desclaux [26], Deutsch *et al.* [28] and Hombourger [12] and Casnati *et al.* [11]. The present EIICS are in good agreement with the data measured by Tawara *et al.* [22] within

5%. The experimental data measured by Glupe and Mehlhorn [27] are overestimated by the present cross sections about $< -20\%$. At high energy the present cross-section lie below the experimental data of Isaacson [23]. The present calculated cross sections are very close to calculated by Kim and Desclaux [26], Hombourger [12] and Casnati *et al.* [11].The results by Deutsch *et al.* [28] seems to be shifted slightly towards left and under estimate in comparison with the all other data.

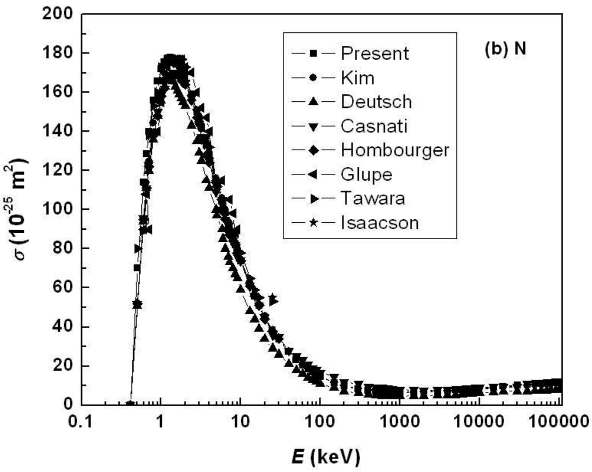

Figure 2: Comparison between the present electron impact ionization cross section and the experimental data for nitrogen (N). ■, the present work; •, theoretical data by Kim and Desclaux [26]; ▲, theoretical data by Deutsch *et al.* [28]; ▼, theoretical data by Casnati *et al.* [11]; ♦, theoretical data by Hombourger [12]; ◄, experimental data by Glupe and Mehlhorn [27]; ►, experimental data by Tawarai *et al.* [22]; ★, experimental data by Isaacson [23].

It is evident from the Fig. 3 that the present theoretical values for O atom are in good agreement with experimental data of Tawara *et al.* [22] within 4%. As it was expected, till $E > 4$ keV the present cross-sections overestimate cross sections measured by Glupe and Mehlhorn [27] and Platten *et al.* [29] about less than 10%. Here we see again that at high energy the present cross-section is lower than those measured by Isaacson [23]. Theoretical EIICS calculated for oxygen by Hombourger [12], Kim and Desclaux [26], Casnati *et al.* [11], Deutsch *et al.* [28].We have also noticed here that the present cross-sections underestimate the cross sections calculated by Kim and Desclaux [26], Hombourger [12] and Casnati *et al.* [11] at low energies while they lie below theoretical cross sections of Deutsch *et al.* [28] at entire energies range. However, the shape of the curve is similar for all five theories. EIICS obtained with our modified formula is reliable in the whole energy range.

4 Conclusion

In this paper, we report comprehensive calculations of K- shell EIICS for light atoms and also compared with the available experimental and theoretical data. Present method has been

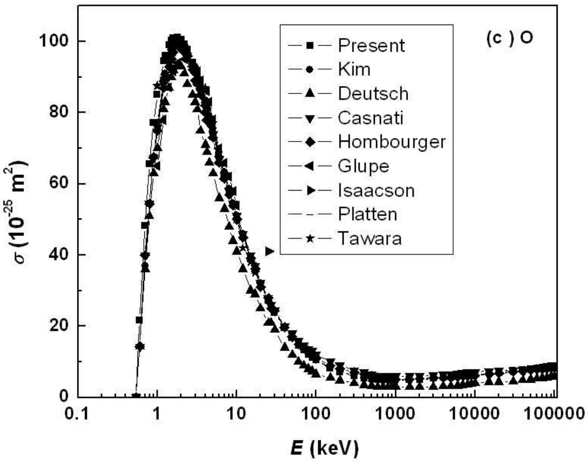

Figure 3: Comparison between the present theoretical electron impact ionization cross section and the experimental data for oxygen (O). ■, present work; •, theoretical data by Kim and Desclaux [26]; ▲, theoretical data by Deutsch *et al.* [28]; ▼, theoretical data by Casnati *et al.* [11]; ⧫, theoretical data by Hombourger [12]; ◄, experimental data by Glupe and Mehlhorn [27]; ►, experimental data by Isaacson [23]; −−−, experimental data by Platten *et al.* [29]; ★, experimental data by Tawarai *et al.* [22].

successfully tested for a number of molecular targets [30].We have investigated EIICS for carbon, nitrogen and oxygen atom in the incident energy region from ionization threshold to 1 GeV. Furthermore we concluded the extended Khare [18] model which has considerably improved the agreement between the experimental and theoretical data for entire energy range. The values of $F(x)$ are fitted by the Eq. (11), on reliable measured EIICS for light atomic series. The obtained results by the extended model achieve a level of agreement with experimental data those are better than the predictions from the previous empirical and semi empirical methods over the wide incident energies. As far as we know there is no other single model to apply for such a wide range of energies and seems to be very use full for applications.

In future, the present model is to extend the calculations to other heavy targets and to inner atomic shells is in progress. Dissociative ionization of molecules is also desirable to calculate.

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