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K-Shell Ionization Cross Sections of Arsenic and Yttrium by electron impact

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Abstract

The total cross sections for K-shell ionization of targets, Arsenic and Yttrium (i.e., As & Y), have been calculated due to electron impact at the incident electron energy from ionization threshold to 1 GeV by using the theoretical Khare method modified by Y Kumar *et al*.[3]. This method is based on plane wave Born approximation. The calculated cross sections have been compared with the available experimental data and other theoretical cross sections. The present calculated cross sections are in excellent agreement with measured by Merlet C. *et al*. [15] and Hoffmann *et al*.[22] for As. A good agreement is found between the present calculations and measured Luo Z. *et al*.[21], Ishii K. *et al*.[23] for Y.

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Key words : Ionization cross section; Atoms; Electron impact; K-shell.

Introduction

The electron impact ionization cross sections have important applications in fields such as mass spectrometry, radiation science, semiconductor physics, atmosphere physics, astrophysics, x-ray laser and fusion research[1-3]. The ionization cross sections by electron impact for K-shell ionization are needed for modeling of radiation effects in materials, in biomedical research and modeling of fusion plasmas in tokomaks. They are also used for material analysis by electron probe micro-analysis (EPMA), surface analysis by Augerelectron spectroscopy (AES) and thin film characterization by electron loss spectroscopy (EELS). Nevertheless, despite more than seven decades of effort by many scientists, there is still inadequate experimental and theoretical knowledge of the dependence of the cross section for ionization of different inner subshell on atomic number and electron kinetic energy.

Many theoretical and experimental studies have been carried out to estimate the electron impact K-shell ionization cross section by various groups. First of all, the classical formula for K-shell ionization is given by Gryzinski, 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.*[4] for atomic ionization cross sections covering the whole energy range. Their formula uses a weighted sum of the squared radii of the maximum charge density of the electron subshells. The final expression involves a number of parameters which are different for s, p and d bound electrons and 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)[6] and Distorted Wave Born Approximation (DWBA)[7] came to light. Recently, LIovet *et al.*[8] have used the formulation of the distorted-wave Born approximation by Bote and Salvat[7] to generate the ionation cross sections of the inner shells by electron impact. Powell[9] reviewed the available calculations, measurements and predictive formulae for inner shell ionization cross sections and presented an analysis of the data in terms of the Bethe equation for the ionization cross sections.

In ultrarelativistic energy region, Scofield[10] 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 ultrarelativistic energies. However, these methods fail at impact energies near the threshold of ionization. Homobourger *et al.*[11] 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.*[12] have developed analytical formulae, referred as BELL formulae, involving species-dependent parameters. Casnati *et al.*[13] proposed another empirical model to describe cross sections for ($6 < Z < 79$).

Khare *et al.*[6] have calculated the electron impact ionization cross sections for K-shell for a number of atoms. They have employed the Plane Wave Born Approximation (PWBA) with corrections for exchange, coulomb, and relativistic effects. In 2000 Kim *et al.*[14] proposed the relativistic version of the BEB model and calculated the cross sections for K-shell ionization of atoms by using their relativistic BEB formula. Many researchers like Haque *et al.*[15], Uddin *et al.*[16], Patoatry *et al.*[17], Huo *et al.*[18], Talukder *et al.*[19] etc. have calculated the K shell ionization cross sections by modified the different model from threshold to ultra-relativistic energy range.

Experimentally, many researchers, Ref. [20-26] have measured the ionization cross sections for K-shell for a number of atoms by electron impact in last five decades.

In 1999 Khare *et al.*[27] 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 Plane Wave Approximation (PWBA)[28] and Binary-Encounter-Bethe [BEB] model of Kim *et al.*[29], where $(1-w/E_r)$ was replaced by $E_r/(E_r+I+U)$, w is the energy loss 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 the 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 *et al.*[29]. Following Kim *et al.*[29], they have used the COOS $df/dw = NI/w^2$ and dropped the contribution of exchange to Bethe term. Although Bethe and Mott cross-sections in Khare *et al.*[29] model are different corresponding cross-sections of Kim [BEB] model but the total ionization cross sections obtained in both model are very close to other. The Khare [BEB] is modified by Y. Kumar[30] by replacing the acceleration I+U by $I = I\left[\frac{1}{1+F}\right]$, F is fitted by the equation F= ξ Z, Where ξ=.018 and *h*=1.77 are fitting parameter for k shell ionization.

In the present investigation, we have used modified Khare model *et al*.[30] to calculate the total cross sections for K-shell ionization of Arsenic and Yttrium atoms due to electron impact at the incident electron energy from ionization threshold to 1 GeV.

Theory :

In modified Khare [BEB] model[30], the ionization cross section is given by

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

Where Bethe cross section

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

Mott cross section

$$\sigma_{PMB} = \left[\frac{s}{t+f}\right]\left[\left(1-\frac{2}{t+1}+\frac{t-1}{2t^2}\right)+\left(\frac{5-t^2}{2(t+1)^2}-\frac{1}{t(t+1)}\right)-\left(\frac{(t+1)}{t^2}\ln\left(\frac{t+1}{2}\right)\right)\right] \tag{3}$$

and the cross section due to the transverse interaction is

$$\sigma_t = -\frac{SI_r^2}{NR(t+f)} M^2 \left\{\ln\left(1-\beta^2\right)+\beta^2\right\} \tag{4}$$

$$t = \frac{E_r}{I_r} \qquad S = \frac{4\pi R^2 N a_0^2}{I_r^2}$$

Here R is the Rydberg energy. β is the ratio of the incident velocity v, and the velocity of light c and M^2 is equal to the total dipole matrix squared for the ionization. It is given by

$$M^2 = \int_{Inl}^{W\max} \frac{R}{W} \frac{df(W,0)}{dW} dW \tag{5}$$

For the incident electron of the rest mass m and velocity v, the relativistic energy E_r is given by

$$E_r = \frac{1}{2}mv^2 = \frac{1}{2}mc^2\left[1-\frac{1}{\left(1+\frac{E}{mc^2}\right)^2}\right] \tag{6}$$

&

$$I_r = \frac{1}{2} m v_b^2 = \frac{1}{2} mc^2 \left[1 - \frac{1}{\left(1 + \frac{I}{mc^2}\right)^2} \right] \qquad (7)$$

Where I_r is the kinetic energy of an electron with speed v_b and I is the binding energy, and

$$f = \left[\frac{h}{1+F} \right]$$

F is fitted by the equation

$$F = \xi Z,$$

Where ξ =.018 and h=1.77 are the fitting parameters for k shell ionization[2].

Bethe collision parameter (b_{nl}) is defined by

$$b_{nl} = \frac{I_{nl}}{Z_{nl}} \int_0^{W_{max}} \frac{1}{W} \frac{df(W,0)}{dW} dW \qquad (8)$$

Where Z_{nl} is the number of electrons present in the (*nl*) subshell of the atom.
From equation (5) and (8) we get the relation between M^2 and Bethe collision parameter (b_{nl})

$$b_{nl} = \frac{I_r M^2}{Z_{nl} R} \qquad (9)$$

Taking $Z_{nl} = N$ and putting the value of M^2 from equation (9) in the equation (4), we get

$$\sigma_t = -\frac{S b_{nl}}{(t+f)} \left\{ \ln\left(1-\beta^2\right) + \beta^2 \right\} \qquad (10)$$

With COOS df/dw=NI/w^2 and taking the value of W_{max} = infinite, we get the value of Bethe collision parameter (b_{nl}) is equal to .5 for all atoms that do not depend on *Z*. This is because at present the appropriate form of the COOS is not known. It will be convenient to take the value of the Bethe parameter b_{nl} in the Khare parameters [Ref. 6]. The value of b_{nl} in the Khare parameters is given by

$$b_{nl} = \alpha p^{-\gamma} \qquad (11)$$

Where $p = I/I_s$, $I_s = Z_s^2 R$, $Z_s = Z - s$ is the effective atomic number, s is the screening parameter, and the Khare parameters[33] are α =.285 & γ=1.7 0.
The recoil energy Q_- is given by

$$Q_- = 0.5mc^2 \left[\left\{ E_r \left(Er - \omega \right) \right\}^{\frac{1}{2}} - \left\{ \left(E_r - \omega \right) \left(E_r - \omega + 2mc^2 \right) \right\}^{\frac{1}{2}} \right]^2 \qquad (12)$$

is due to the assumption that a quite large contribution to the integral comes from the small values of ω . Hence for ω << E we obtain from (eq.12)

$$Q_{-} = \frac{\omega^2}{4}\left[\frac{1}{2}mc^2 + \frac{1}{E_r}\right] \tag{13}$$

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

$$\sigma_{PBB} = \left[\frac{s}{t+f}\right]\left[.4431\left(1-\frac{1}{t^2}\right) - 0.5\left(\frac{1}{t} + \frac{I_r}{2mc^2}\right) + \frac{1}{2t^2}\ln\left(1+\frac{E_r}{2mc^2}\right)\right] \tag{14}$$

After putting the values of σ_{PMB}, σ_t and σ_{PBB} from equation (3), (10) and (14) into equation (1) the K-shell ionization cross sections are obtained for the atom.

Results and Discussion

In the present investigation, K-shell ionization cross sections have been calculated for the two atoms, Arsenic and Yttrium by the modified Khare [BEB] model[30] for incident energy varying from threshold ionization energy to high energy (GeV). The ionization potentials are taken from Desclaux[31] and Jolly *et al*.[32]. Recently, Liovet *et al*.[8] have calculated the ionization cross sections in the energy range from threshold ionization to 1 GeV by using Distorted Wave Born Approximation (DWBA) of D Bote and F Salvat[7]. They have emphasized that these results are in good agreement with the experimental results. We have taken only these theoretical calculations to compare the present ionization cross sections.

Figure 1 shows the comparison of present cross- sections for Arsenic along with the experimental data given by Merlet *et al.*[24] and theoretical results of LIovet *et al*.[8] of the ionization cross sections in the energy range from threshold ionization energy to 100 KeV for Arsenic. The present calculations are in outstanding agreement with the experimental data measured by Merlet *et al.*[24] within 5%. The theoretical ionization cross sections calculated by LIovet *et al*.[8] and present ionization cross sections are very close to each other. Figure 2 compares the present calculated ionization cross sections with available experimental data of the Hoffmann *et al.*[22] and theoretical calculations of LIovet *et. al*.[8] in the energy range from 100 KeV to 1 GeV for the Arsenic. The figure shows the excellent agreement with the present calculated ionization cross sections and the experimental data by Hoffmann *et al*.[22] as well as theoretical ionization cross sections calculated by LIovet *et al*.[8].

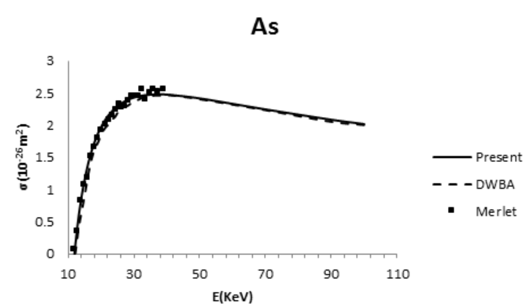

Figure 1 – The solid line and dash line shows present total cross section and theoretical total cross section of DWBA calculations by LIovet *et al*.[8] for K shell of Arsenic, respectively for energy range from threshold ionization energy to 100 KeV. Experimental data are shown by symbol

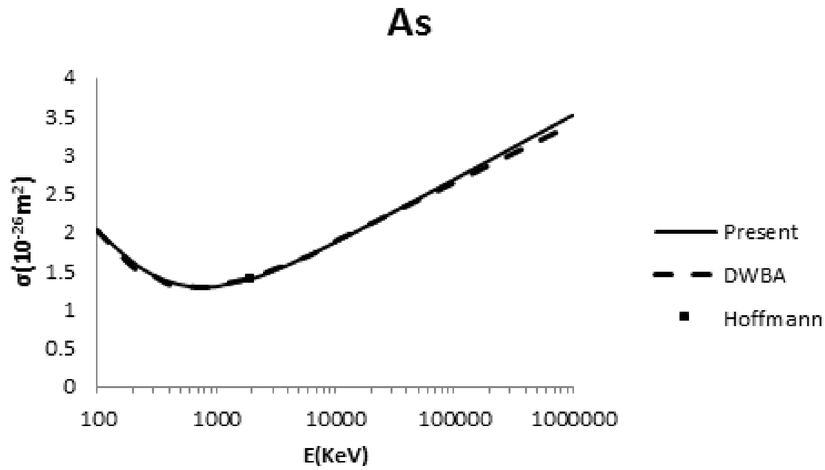

Figure 2 –The solid line and dash line shows present total cross section and theoretical total cross section of DWBA calculations by LIovet *et al.*[8] for K shell of Arsenic energy range from 100 KeV to 1GeV, respectively. Experimental data are shown by symbol. Here logarithmic scale on horizontal axis is used

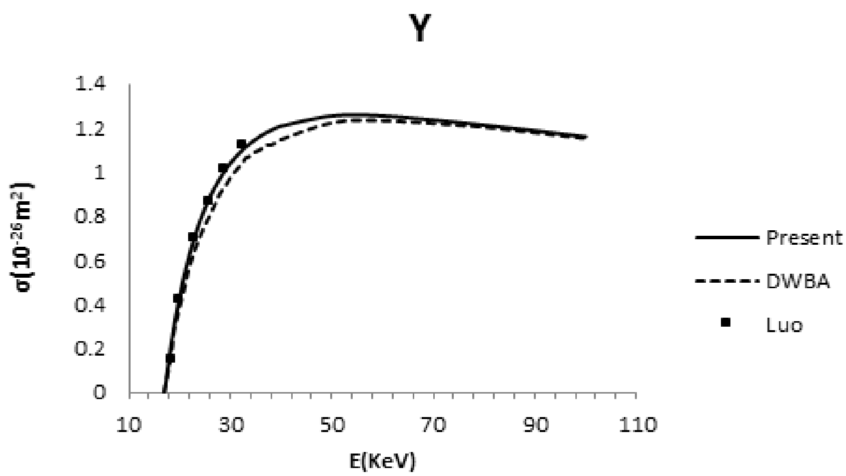

Figure 3 – The solid line and dash line shows present total cross section and theoretical total cross section of DWBA calculations by LIovet *et al.*[8] for K shell of Yttrinium, respectively for energy range from threshold ionization energy to 100 KeV. Experimental data are shown by symbol.

The comparison of present calculated ionization cross sections with the available experimental data, and theoretical ionization cross sections of Liovet *et al.*[8] are shown in figure 3 in the range from threshold ionization energy to 100 KeV for Yttrium. We have only one experimental data measured by Luo *et al.*[20] for this energy range. The present calculated cross sections are in excellent agreement with the experimental data of Luo *et al.*[20]. The present calculations are slighty higher than the theoretical values of LIovet *et al.*[8].

Figure 4 shows the K-shell ionization cross-sections for Yttrium in the energy range from 100 KeV to 1GeV. The present cross-sections agree well with experimental data measured by Ishii *et al.*[21], Hoffmann *et al.*[22] and Berenyi *et al.*[23]. The two theoretical calculations Liovet *et al.*[8] and present calculations are very close to each other.

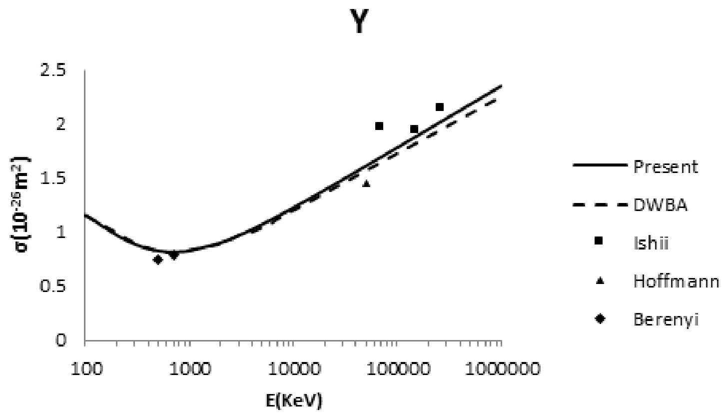

Figure 4 – The solid line and dash line shows present total cross section and theoretical total cross section of DWBA calculations by LIovet *et al*.[8] for K shell of Yttrinium energy range from 100 KeV to 1GeV, respectively. Experimental data are shown by symbol. Here logarithmic scale on horizontal axis is used.

Conclusion

The proposed model, an extension of the Khare *et al*.[27] model for the electron impact ionization of molecules, are examined for K-shell ionization on 2 atomic targets (As and Y) up to ultra-relativistic incident energies. The calculated values of cross sections are compared with the available experimental and theoretical data. We can conclude that a slight modification in Khare et al. model has considerably improved the agreement between the experimental and theoretical data. The primary application of the present model is to extend the calculations to other targets and to inner atomic shells is in progress.

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