K-Shell Ionization Cross Sections of Chromium and Cobalt by electron impact

SACHIN KUMAR¹, MANOJ KUMAR¹, YOGESH KUMAR² and SAKSHI CHAUDHARY³

¹Department Of Physics, Meerut College, Meerut-250001, (India)
²Department Of Physics, D.A.V. College, Muzaffarnagar-251001, (India)
³Department Of Chemistry, D.N. College, Meerut-250001, (India)

Corresponding Author – Sakshi Chaudhary - sakshisachin07@gmail.com
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Abstract

The theoretical Khare model modified by Y Kumar et al. [J. At. Mol. Sci. (2012)], has been used to calculate the total cross sections for K-shell ionization of two targets, chromium, and cobalt, (i.e., Cr & Co) due to electron impact at incident electron kinetic energy from ionization threshold energy to 1 GeV. This method is based on plane wave Born approximation. The present model requires only two atomic parameters, ionization energy, and atomic number. 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 Liovet et al. [J. Phys.B 33, 2000] and Hoffmann et al. [Z. Phys. Rev. A 22, 1980] for Cr. A good agreement is found between the present calculations and measured An et al. [Chin. Phy. Lett. 18, 2001] and Se et al. [Phys. Lett. 29, 1974].

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

Introduction

The ionization cross sections by electron impact find important applications in fields such as mass spectrometry, radiation science, semiconductor physics, atmosphere physics, astrophysics, x-ray laser and fusion research¹³. The computed data on cross sections are necessary for studying the problems of radiative association. The 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. They are also
used for material analysis by electron probe micro-analysis (EPMA), surface analysis by Auger-electron 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 experimental and theoretical 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\(^4\), which provides a fairly good description over a wide energy range except near the threshold region. This formula was further modified by Deutsch \textit{et al.}\(^5\) 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 are different from those given by Gryzinski\(^4\). 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, Llovet \textit{et al.}\(^9\) have used the formulation of the distorted-wave Born approximation by Bote and Salvat\(^7\) to generate the ionization 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 \textit{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 \textit{et al.}\(^12\) have developed analytical formulae, referred as BELL formulae, involving species-dependent parameters. Casnati \textit{et al.}\(^13\) proposed another empirical model to describe cross sections for (6\(<\ Z\ <\ 79\)).

Khare \textit{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 \textit{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 \textit{et al.}\(^15\), Uddin \textit{et al.}\(^16\), Patoatry \textit{et al.}\(^17\), Kumar S and Kumar Y.\(^18\), Talukder \textit{et al.}\(^19\), etc. have calculated the K shell ionization cross sections by modified the different model from threshold to ultrarelativistic 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 \textit{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 \textit{et al.}\(^29\), where \((1-\ w/\ E_r)\) was replaced by \(E_r/\ (E_r+I+U)\), \(w\) 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 et al.\textsuperscript{29}. Following Kim et al.\textsuperscript{29}, they have used the COOS $\frac{df}{d\omega}=NI/w^2$ and dropped the contribution of exchange to Bethe term. Although Bethe and Mott cross-sections in Khare et al.\textsuperscript{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\textsuperscript{30} by replacing the acceleration $I+U$ by $I = I \left[ \frac{1}{1+F} \right]$, F is fitted by the equation $F=\xi Z$, Where $\xi=0.18$ and $h=1.77$ are fitting parameter for k shell ionization.

In the present investigation, we have used modified Khare model et al.\textsuperscript{30} to calculate the total cross sections for K-shell ionization of chromium and cobalt atoms due to electron impact at incident electron energy from ionization threshold to 1 GeV.

**Theory**:

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

$$\sigma_I = \sigma_{PBB} + \sigma_{PMB} + \sigma_t$$ (1)

Where Bethe cross section

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

Mott cross section

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

and the cross section due to the transverse interaction is

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

$$t = \frac{E_r}{I_r}, \quad S = \frac{4\pi R^2 Na_0^2}{I_r^2}$$

Here R is the Rydberg energy, $\beta$ 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

$$M^2 = \int_{W_{\text{max}}} W \frac{df(W,0)}{dW} dW$$ (5)

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

$$E_r = \frac{1}{2}mv^2 = \frac{1}{2}mc^2 \left[ 1 - \frac{1}{\left( 1 + \frac{E}{mc^2} \right)^2} \right]$$ (6)
\[ I_r = \frac{1}{2} m v_b^2 = \frac{1}{2} m c^2 \left[ 1 - \frac{1}{\left( 1 + \frac{I}{mc^2} \right)^2} \right] \]  

(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 \( \xi = 0.018 \) and \( h = 1.77 \) are the fitting parameters for k shell ionization.²

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

\[ b_{nl} = \frac{I_{nl} \left( f \right)}{Z_{nl}} \int_0^{W_{nl}} \frac{df(W,0)}{W} dW \]

(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 \( (b_{nl}) \)

\[ b_{nl} = \frac{I_{nl} M^2}{Z_{nl} R} \]

(9)

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

\[ \sigma_{22} = -\frac{S b_{nl}}{(r + f)} \left\{ \ln \left( 1 - \beta^2 \right) + \beta^2 \right\} \]

(10)

With COOS \( df/d\omega = NI/\omega^2 \) and taking the value of \( W_{\text{max}} = \infty \), 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

\[ b_{nl} = \alpha p^{-\gamma} \]

(11)

Where \( p = I/I_s, I_s = \frac{Z_{\alpha}^2}{R}, Z_{\alpha} = Z - s \) is the effective atomic number, \( s \) is the screening parameter, and the Khare parameters³³ are \( \alpha = 0.285 \) & \( \gamma = 1.70 \).

The recoil energy \( Q \) is given by

\[ Q = 0.5mc^2 \left[ \left\{ E_r \left( E_r - \omega \right) \right\}^{1/2} - \left\{ (E_r - \omega) (E_r - \omega + 2mc^2) \right\}^{1/2} \right]^2 \]

(12)

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

$$Q = \frac{\omega^2}{4} \left[ \frac{1}{2} mc^2 + \frac{1}{E_f} \right]$$

(13)

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

$$\sigma_{PBB} = \left[ \frac{s}{t + f} \right] \left[ 0.4431 \left( 1 - \frac{1}{t^2} \right) - 0.5 \left( \frac{1}{t} + \frac{I_f}{2mc^2} \right) + \frac{1}{2t^2} \ln \left( 1 + \frac{E_f}{2mc^2} \right) \right]$$

(14)

After putting the values of $\sigma_{PMB}, \sigma_t$ and $\sigma_{PBB}$ 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 the K-shell ionization cross sections have been calculated for the two atoms, chromium and cobalt by the modified Khare [BEB] model for incident energy varying from threshold ionization energy to high energy (GeV). The ionization potentials are taken from Desclaux and Jolly et al. Recently, Liovet et al. 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. 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 chromium along with the experimental data given by various groups and theoretical results of Liovet et al. of the ionization cross sections in the energy range from threshold ionization energy to 100 KeV for chromium. Except for low energies, the present calculations are in excellent agreement with the experimental data measured by Liovet et al. within 10%. The experimental data, measured by He et al. lie below the present ionization cross sections. However, the measured values of An et al. are underestimated by the present calculations. It is evident from the figure that the present calculated ionization cross sections are in good agreement with experimental data of Luo et al. The theoretical ionization cross sections calculated by Liovet et al. and present ionization cross sections are very close to each other.

![Figure 1](image)

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. for K shell of chromium, respectively for energy range from threshold ionization energy to 100 KeV. Experimental data are shown by symbol.
Figure 2 compares the present calculated ionization cross sections with available experimental data of the Scholz et al.\textsuperscript{24} and Hoffmann et al.\textsuperscript{25} and theoretical calculations of Llovet et. al.\textsuperscript{7} in the energy range from 100 KeV to 1 GeV for the chromium. The present calculated ionization cross sections are agreed with the experimental data by Hoffmann et al.\textsuperscript{25} within 5%. Scholz et al.\textsuperscript{24} have measured the ionization cross sections at 2000 KeV, which is overestimated by the present calculations.

![Cr Cross Section](image1)

**Figure 2** – The solid line and dash line shows present total cross section and theoretical total cross section of DWBA calculations by Llovet et al.\textsuperscript{7} for K shell of chromium energy range from 100 KeV to 1 GeV, respectively. Experimental data are shown by symbol. Here logarithmic scale on horizontal axis is used.

![Co Cross Section](image2)

**Figure 3** – The solid line and dash line shows present total cross section and theoretical total cross section of DWBA calculations by Llovet et al.\textsuperscript{7} for K shell of cobalt, respectively for energy range from threshold ionization energy to 100 KeV. Experimental data are shown by symbol.

![Co Cross Section](image3)

**Figure 4** – The solid line and dash line shows present total cross section and theoretical total cross section of DWBA calculations by Llovet et al.\textsuperscript{7} for K shell of cobalt, respectively energy range from 100 KeV to 1 GeV. Experimental data are shown by symbol. Here logarithmic scale on horizontal axis is used.
In figure 3 the present cross sections for cobalt are compared with the experimental data of An et al.\textsuperscript{26} and theoretical cross sections of Liovet et al.\textsuperscript{7} in the energy range from threshold ionization energy to 100 KeV. The agreement between the experimental data and the present results is quite good with 5%.

At low energies the present calculations are very close to calculated cross sections of Liovet et al.\textsuperscript{7}, however, for the energies higher than the 20 KeV present values of cross section lie below the calculated cross sections of Liovet et al.\textsuperscript{7}.

The comparison of present calculated ionization cross sections with the available experimental data Scholz et al.\textsuperscript{24} and theoretical ionization cross sections of Liovet et al.\textsuperscript{7} are shown in figure 4 in the energy range from 100 KeV to 1 GeV for cobalt. In this range, the present calculated ionization cross sections agree with these experimental data of Scholz et al.\textsuperscript{24} and theoretical calculations of Liovet et al.\textsuperscript{7}.

Conclusion

The proposed model, an extension of the Khare et al.\textsuperscript{27} model for the electron impact ionization of molecules, are examined for K-shell ionization on 2 atomic targets (Cr and Co) up to ultra-relativistic incident energies. The calculated cross sections are compared with the available experimental and theoretical data. We conclude that a slight modification in Khare et al.\textsuperscript{27} model have considerably improved the agreement between the experimental and theoretical data. The application of the present model is to extend the calculations to other targets and to inner atomic shells is in progress. This constitutes the future scope for the present model.

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