



(Print)

JUSPS-A Vol. 30(4), 257- 264 (2018). Periodicity-Monthly

Section A

(Online)



Estd. 1989

JOURNAL OF ULTRA SCIENTIST OF PHYSICAL SCIENCES
An International Open Free Access Peer Reviewed Research Journal of Mathematics
website:- www.ultrascientist.org

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

<http://dx.doi.org/10.22147/jusps-A/300404>

Acceptance Date 05th March, 2018,

Online Publication Date 2nd April, 2018

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. Phys. Lett. 18, 2001] and Se *et al.* [Phys. Lett. 29, 1974].

PACS No — 34.80Dp

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 research¹⁻³. 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 Gryzinski⁴, 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.*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 Gryzinski⁴. 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 *et al.*⁹ have used the formulation of the distorted-wave Born approximation by Bote and Salvat⁷ to generate the ionization cross sections of the inner shells by electron impact. Powell⁹ 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, Scofield¹⁰ 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, Kumar S and Kumar Y.¹⁸, Talukder *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 *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 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. Kumar³⁰ 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 $\xi = 0.018$ 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 chromium and cobalt atoms due to electron impact at incident electron energy from ionization threshold to 1 GeV.

Theory :

In modified Khare [BEB] model³⁰, the ionization cross section is given by

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

Where Bethe cross section

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

Mott cross section

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

and the cross section due to the transverse interaction is

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

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

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

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

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

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

&

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

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 $\xi = .018$ and $h = 1.77$ are the fitting parameters for k shell ionization².

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

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

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})

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

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

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

With COOS $df/dw = NI/w^2$ and taking the value of $W_{\max} = \infty$, 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

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

Where $p = I/I_s$, $I_s = \frac{Z_s^2}{8} R$, $Z_s = Z - s$ is the effective atomic number, s is the screening parameter, and the Khare parameters³³ are $\alpha = .285$ & $\gamma = 1.70$.

The recoil energy Q is given by

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

is due to the assumption that a quite large contribution to the integral comes from the small values of ω . Hence

for $\omega \ll E$ we obtain from (eq.12)

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

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

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

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 the K-shell ionization cross sections have been calculated for the two atoms, chromium and cobalt by the modified Khare [BEB] model³⁰ for incident energy varying from threshold ionization energy to high energy (GeV). The ionization potentials are taken from Desclaux³¹ and Jolly *et al.*³². Recently, Llovet *et al.*⁷ 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 Salvat⁶. 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 Llovet *et al.*⁷ 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 Llovet *et al.*²⁰ within 10%. The experimental data, measured by He *et al.*²¹ lie below the present ionization cross sections. However, the measured values of An *et al.*²² 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.*²³. The theoretical ionization cross sections calculated by Llovet *et al.*⁷ and present ionization cross sections are very close to each other.

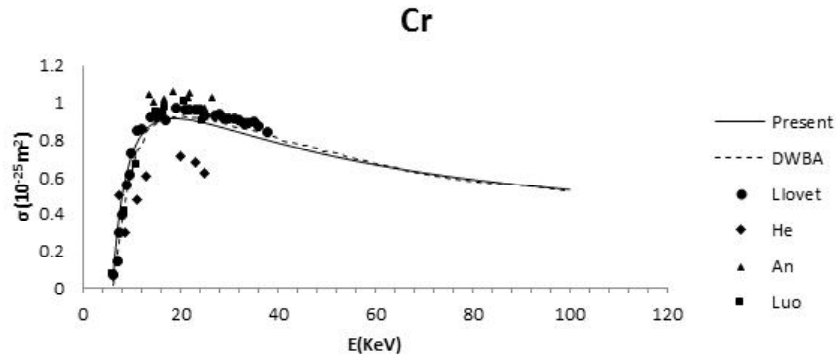


Figure 1 – The solid line and dash line shows present total cross section and theoretical total cross section of DWBA calculations by Llovet *et al.*⁷ for K shell of chromium, respectively for energy range from threshold ionization energy to 100 KeV. Experimental data are shown by symbol.

Figure 2 compares the present calculated ionization cross sections with available experimental data of the Scholz *et al.*²⁴ and Hoffmann *et al.*²⁵ and theoretical calculations of Llovet *et al.*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.* [25] within 5%. Scholz *et al.* [24] have measured the ionization cross sections at 2000 KeV, which is overestimated by the present calculations.

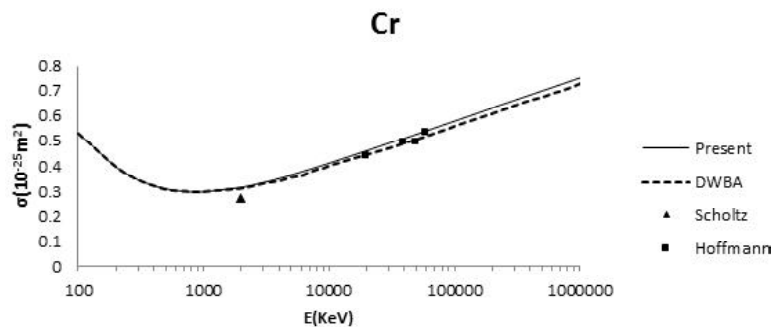


Figure 2 –The solid line and dash line shows present total cross section and theoretical total cross section of DWBA calculations by Llovet *et al.*⁷ for K shell of chromium energy range from 100 KeV to 1GeV, respectively. Experimental data are shown by symbol. Here logarithmic scale on horizontal axis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

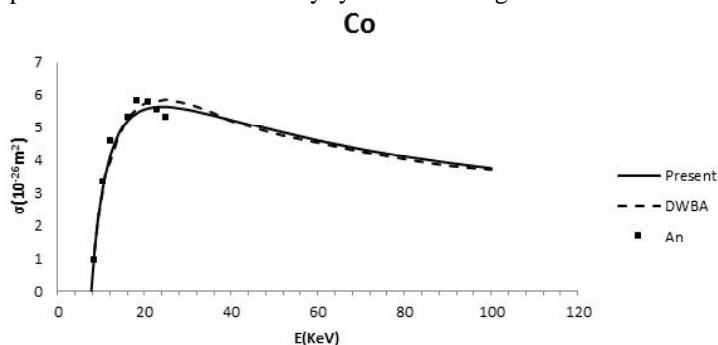


Figure 3 – The solid line and dash line shows present total cross section and theoretical total cross section of DWBA calculations by Llovet *et al.*⁷ for K shell of cobalt, respectively for energy range from threshold ionization energy to 100 KeV. Experimental data are shown by symbol.

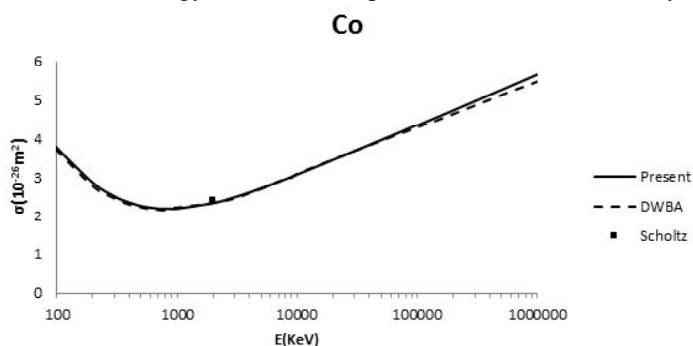


Figure 4 – The solid line and dash line shows present total cross section and theoretical total cross section of DWBA calculations by Llovet *et al.*⁷ for K shell of cobalt, respectively energy range from 100 KeV to 1GeV. Experimental data are shown by symbol. Here logarithmic scale on horizontal axis is used.

In figure 3 the present cross sections for cobalt are compared with the experimental data of An *et al.*²⁶ and theoretical cross sections of Llovet *et al.*⁷ in the energy range from threshold ionization energy 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 Llovet *et al.*⁷, however, for the energies higher than the 20 KeV present values of cross section lie below the calculated cross sections of Llovet *et al.*⁷.

The comparison of present calculated ionization cross sections with the available experimental data Scholz *et al.*²⁴ and theoretical ionization cross sections of Llovet *et al.*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.*²⁴ and theoretical calculations of Llovet *et al.*⁷.

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 (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.*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.

Acknowledgement

Authors are grateful to the principal, meerut college, meerut, which gave us financial support and facilities for our research work. Authors are also grateful to Ex. Professor S. P. Khare of C.C.S. University, Meerut, India for many fruitful discussions.

References

1. Shalenov E.O., Dzhumagulova K. N. and Ramazanov T.S. "Scattering cross sections of the particles in the partially ionized dense nonideal plasmas" Phys. Plasmas 24, 012101 (2017).
2. Irikura K K, "Partial ionization cross section of organic molecules" J. Res. Natl. Inst. Stan. 122, 1-67 (2017).
3. Kim C.G., Jung Y.D. "Quantum dynamic screening effects on the elastic collisions in strongly coupled semiclassical plasmas", Plasmas 19, 014502-014509 (2012).
4. Gryzinski M. "classical theory of collisions" Phys. Rev. 138, A336-358, (1965).
5. Duetsch H, Becker K and Mark T D, "calculated cross sections for the electron-impact ionization of m atoms" Int. J Mass Spectrom. 177, 47 (1998).
6. Khare S P, Saksena V. and Wadehra J M "K-shell ionization of atoms by electron and positron impact" Phys. Rev. A 48, 1209-1213 (1993).
7. Bote D and Salvat F, "Calculations of inner-shell ionization by electron impact with the distorted-wave and plane-wave Born approximation" Phys. Rev. A 77, 042701 (2008).
8. Llovet X, Powell C J, Salvat F and Jablonski A, "Cross section for inner shell ionization by electron impact" J. Phys. Chem. Ref. Data, Vol. 43 No. 1, 013102-61 (2014).
9. Powell C L "inner shell ionization cross sections", Rev. Mod. Phys., 48, 33-47 (1976).
10. Scofield J H "K- and L-shell ionization of atoms by relativistic electrons," Phys Rev A, 18, 963-970 (1978).
11. Hombourger C "An empirical expression for K-shell ionization cross section by electron impact" J. Phys.

- B 31, 3693-3702 (1998).
12. Bell K L, Gilbody H B, Hudhes J G, Kingston A E and Smith F J, "Recommended Data on the Electron Impact Ionization of Light Atoms and Ions" Phys Chem Ref Data, 12, 891 (1983).
 13. Casnati Etartari A and Baraldi C "An empirical approach to K shell ionization cross section by electron" J. Phys. B At. Mol. Phys. 15, 155-167 (1982).
 14. Kim Y.K., Santos J P and Parente F. "Extension of the binary-encounter-dipole model to relativistic incident electron" Phys. Rev A 62 052710 (2000).
 15. Haque A K F, Uddin M A, Basak A K, Karim K R, Saha B C and Malik F B "Generalized Kolbensvedt for electron impact ionization of the K-, L- and M-shell ions", Phys Rev A, 73, 012708 (2006).
 16. Uddin M A, Haque A K F, Karim K R, Basak A K and Malik F B "Modified Kolbensvedt for electron impact K-shell ionization cross sections of atoms and ions" Eur Phys J D, 37, 361-369 (2006).
 17. Patoary M A R, Uddin M A, Haque A K F, Basak A K, Talukder M R, Karim K R and Saha B C "Electron impact K-shell ionization cross sections of atoms at relativistic energies" Int. J. Quantum Chem. 108, 1023 (2007).
 18. Kumar S and Kumar Y. "K-shell ionization cross sections of alkali metals by electron impact", IJP, 1, 41-48 (2013).
 19. Talukder M R, Bose S and Taka mura S. "Calculated electron impact K-shell ionization cross sections for atoms" Int. J M S, 269, 118 (2008).
 20. Llovet X, Merlet C and Savlat F "Measurement of K-shell ionization cross sections of Cr, Ni and Cu by impact of 605-40 KeV" J. Phys.B 33, 3761-3772 (2000).
 21. He F Q, Peng X F, Long X G, Luo Z M and An Z "K-shell ionization cross sections by electron bombardment at low energies" Nucl. Instrum. Methods Phys. Res. B 129, 445-450 (1997).
 22. An Z, Li T H, Wang L M, Xia X Y and Luo Z M, "correction of substrate effect in the measurement of 25-KeV electron impact K-shell ionization cross sections of Cu and Co elements", Phys. Rev. 54, 3067-3069 (1991).
 23. Luo Z M, An Z, Li T H, Wang L M, Zhu and Peng. X F "Correction of the influence of the substrate upon the measurement of the K-shell ionization cross sections", Phys. Rev. Lett. 71, 2701-2109 (1993).
 24. Scholz W, Scholz Li A, Colle R and Preiss I L, "K-shell ionization cross section for 20.4-MeV electrons" Phys. Lett. 29, 761-766 (1974).
 25. Hoffmann D H H, Brendel C, Low W Muller S and Ritcter A "inner shell ionization by relativistic electron impact", Z. Phys. Rev. A 22, 413-420 (1980).
 26. An Z, Tang C. H, and Luo Z M "Measurement of K-shell ionization cross sections of Cr, Ni and Cu atoms by 7.5-25 KeV electron impact", Chin. Phy. Lett. 18, 1460-1462 (2001).
 27. Khare S.P., Sharma M.K. and Tomar S. "electron impact ionization of methane" J. Phys. B At. Mol. Opt. Phys. 32, 3147 (1999).
 28. Saksena V., Kushwaha M.S. and Khare S.P. "ionization cross sections of molecules due to electron impact", Physica B233 201 (1997).
 29. Kim Y.K. and Rudd M.E. "Binary-encounter-dipole model for electron-impact ionization" Phys. Rev A50. 3954-67 (1994).
 30. Y. Kumar, N. Tiwari, M. Kumar and S. Tomar. "K-shell ionization cross sections of transition and non transition metal by electron impact" J. At. Mol. Sci. 122 (2012).
 31. Jolly W L, Bomben K D and Eyermann C J, At. Data Nucl. Data Tables 31, 411 (1984).
 32. Desclaux J P At Nucl. Data tables, XII, 325 (1973).
 33. Introduction to the theory of collisions ot electrons with atoms and molecules "S.P. Khare, Klumer Academic Press, New York.