Electron Impacts on K-SHELL Ionization of Alkali Metals

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Abstract: The theoretical modified Khare model et al. [1-2], has been used to calculate the total cross sections for K-shell ionization of 3 targets (Na, K, Rb) 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.

Key Word: Ionization Cross Section; Atoms; Electron Impact; K-Shell.

I. 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 photon, 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 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. First of all, the classical formula for Kshell 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. [3] for atomic ionization cross sections covering the whole energy range. Their formula usesK-Shell Ionization Cross Sections of Alkali Metals by Electron Impactsweighted sum of the squared radii of the maximum charge density of the electron subshells. The final expression involes a number of parameters which are defferent 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 intolight.

In ultrarelativistic 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 ultrarelativistic energies. However, these methods fail at impact energies near threshold of ionization. Homobourger et al. (8) calculated the K shell ionization cross sections by proposing a relativistic empirical expression through an analysis of experimental data for atoms ($6 \le Z \le 76$). 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 Plane Wave Born Approximation (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, 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 et al. [17], Talukder et al. [18] etc. have calculated the K shell ionization cross sections by modified the different model from threshold to ultrarelativisticenergy range.

Experimentally, many researchers, Ref. [22-44] have measured the ionization cross sections for K-shell for a numbers of atoms by electron impact in last five decades.

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 Plane Wave Approximation (PWBA)[19]and Binary-Encounter-Bethe [BEB] model of Kim et al. [12], where $(1-w/E_T)$ was replaced by $E_T/(E_T + I+U)$, w is the energy lose suffered by incident electron in the ionizing collision, E_T 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. [12]. Following Kim et al. [12], 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. [1] model are different corresponding cross-sections of Kim [BEB] model but the total ionization cross sections obtained in both model are very close toother.

In present investigation we have used modified Khare model et al. [2] to calculate the total cross sections for K-shell ionization of alkali atoms due to electron impact at incident electron energy from ionization threshold to 1 GeV.Sachin Kumar and Yogesh Kumar

II. Results and Discussion

In the present investigation the K-shell ionization cross sections have been calculated for the three atoms by modifying the Khare [BEB] model [1] for incident energy varying from threshold ionization energy to high energy (GeV). The ionization potentials are taken from Desclaux [20] and Jolly et al. [21]. Theoretical cros sections, calculated by Hombourger et al. [8], Casnati et al. [10], Kim et al. [11], Uddin et al.

[15] are shown in fig. Figure 1 shows the comparison of present cross- sections for sodium along with the experimental data given by Kamiya et al. [35] and theoretical results of Talukder et al. [18]. Near at 10 KeV present cross sections are slightly lower than the calculated by Talukder et al.[18]. For K shell good agreement between the theory and experimental results for electron impact ionization cross sections has been obtained for Na atom over the wholerange.

E (KeV)



Figure 1

This figure showing the comparison of the present theoretical total cross section to experimental data for Sodium







This figure showing the comparison of the present theoretical total cross section to experimental data for Potasium.



This figure showing the comparison of the present theoretical total cross section to experimental data for Rubidium Figure 2 shows the K-shell ionization cross-sections for Potasium. The theoretical cross sections obtained by Talukder et al. [18] has a tendency overestimates the experimental data up to range 10 KeV, While then underestimates the experimental values up to 100 KeV. The present cross- sections agree well with experimental data measured by Hoffman et al. [27], Schevelko et al. [43] and Ishii et al. [32]

In fig.3 the present cross sections for Rb are compared with the experimental data of Scholz et al. [38] and Schevelko et al. [43]. The figure shows that the agreement between the experimental data and the present results is quite good.

III. Conclusion

The proposed model, an extension of the Khare et al. [1] model for the electron impact ionization of molecules, are examined for K-shell ionization on 3 atomic targets (Na, K, Rb) up to ultrarelativistic 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. 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 inprogress.

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