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Electron impact ionization of Ba, Ba^+ and Ba^{2+}

GOPALJEE, S K SHRIVASTAVA and B N ROY
Department of Physics, B R Ambedkar Bihar University, Muzaffarpur 842 001, India

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Abstract. The binary encounter approximation has been used to investigate the effect of charge state of the target atom (ion) on the electron impact excitation autoionization cross-sections. Roothan–Hartree–Fock (RHF) velocity distribution for the bound electrons has been used throughout the calculations. The present results give a good account of the experimental observations.

Keywords. Electron impact ionization; binary encounter approximation; excitation-autoionization; Roothan–Hartree–Fock velocity distribution.

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1. Introduction

Collisions involving electrons with atoms and ions are one of the most fundamental interactions in physics. These events are basic to a variety of processes such as plasma physics, radiation physics and astrophysics. Electron-impact is also the most common form of ionization in commercial mass spectrometers and is used as an analytical tool for measuring species concentrations in gaseous samples. Total ionization cross-sections are necessary data in modelling and understanding the various environments.

Excitation-autoionization and resonant excitation double autoionization processes are the important indirect physical mechanisms for ionization which received considerable theoretical and experimental attention in recent years. In the excitation-autoionization, an inner shell electron is excited to a level above the ionization threshold which can subsequently decay by autoionization. The inner shell excitation can cause significant rise in the ionization function near the excitation threshold [1–4].

We have used the binary encounter (BE) description of excitation-autoionization contributing to the electron impact ionization [5, 6] for systems Ba, Ba^+ and Ba^{2+}. Systematic studies of these systems may provide some generalization for the dependence of excitation-autoionization on the charge state of the target system.

In quantal approximations, it is difficult to investigate ionization due to the involvement of a large number of states that are to be taken in mathematical formulations. In fact, usually, excitation cross-sections are calculated in different quantal approximations and then added either to the scaled ionization cross-sections of McGuire (7) or to the cross-sections obtained using semiempirical formulae of Lotz [8, 9 see also 10–12]. On the other hand, the binary encounter approximation (BEA) in the case of electron impact ionization of atoms and ions, is quite suitable for the reliable estimation of ionization cross-sections for atoms and ions [5, 6].

In the present work Vriens' [13] expressions for electron impact ionization and excitation cross-sections including exchange and interference have been used throughout the calculations. The effect of the residual ionic field of the target ions (in the case of ions) has been incorporated along the line suggested by Thomas and Garcia [14] [see also 15, 5].

2. Theoretical consideration

Following Gopaljee *et al* [6] (and references therein), Vriens' expressions for electron impact ionization and excitation cross-sections incorporating the effect of residual ionic field of target ion can be written in terms of dimensionless variables,

$$Q_i(s,t)=\frac{(s+s')^2}{s^2(s'^2+t^2+1)}\left[\frac{s'^2-1}{U^2s'^2}+\frac{2t^2}{3}\left(\frac{s'^2-1}{U^2s'^4}\right)-\frac{\varphi'}{U^2(s'^2+1)}1_n s'^2\right](\pi a_0^2) \tag{1}$$

and

$$\begin{aligned}Q_E(s,t)&=\frac{(s+s')^2}{s^2(s'^2+t^2+1)}\left[\frac{1}{U}\left(\frac{1}{U_n}-\frac{1}{U_{n+1}}\right)+\frac{2}{3}t^2\left(\frac{1}{U_n^2}-\frac{1}{U_{n+1}^2}\right)\right.\\&\quad+\frac{1}{U}\left(\frac{1}{s'^2U+U-U_{n+1}}-\frac{1}{s'^2U+U-U_n}\right)\\&\quad+\frac{2}{3}t^2\left(\frac{1}{(s'^2U+U-U_{n+1})^2}-\frac{1}{(s'^2U+U-U_n)^2}\right)\\&\quad\left.-\frac{\varphi''}{(s'^2+1)U}l_n\left(\frac{U_{n+1}(s'^2u+U-U_n)}{U_n(s'^2U+U-U_{n+1})}\right)\right](\pi a_0^2),\quad s'^2U\geqslant U_{n+1}\\&=\frac{(s+s')^2}{s^2(s'^2+t^2+1)}\left[\frac{1}{U}\left(\frac{1}{U_n}-\frac{1}{s'U}\right)+\frac{2}{3}t^2\left(\frac{1}{U_n^2}-\frac{1}{(s'^2U)^2}\right)\right.\\&\quad+\frac{1}{U}\left(\frac{1}{U}-\frac{1}{s'^2U+U-U_n}\right)+\frac{2}{3}t^2\left(\frac{1}{U^2}-\frac{1}{(s'^2U+U-U_n)^2}\right)\\&\quad\left.-\frac{\varphi''}{(s'^2+1)U}l_n\left(\frac{s'^2(s'^2U+U-U_n)}{U_n}\right)\right](\pi a_0^2),\quad U_n\leqslant s'^2U\leqslant U_{n+1}.\end{aligned} \tag{2}$$

The expressions for ionization and excitation cross-sections have been integrated over the Roothan–Hartree–Fock velocity distribution for the bound electrons. Roothan–Hartree–Fock radial functions given by McLean and McLean [16] have been used to construct the momentum distribution function. In case of Ba^{2+}, due to non-availability of RHF radial functions, hydrogenic velocity distribution has been used. For the calculation of ionization and excitation cross-sections, in the case of Ba, the modifications made in Vriens' expressions (1) and (2) to incorporate the effect of residual ionic field of the target ion have been dropped off.

In excitation-autoionization calculations, as there is usually abrupt increase in cross-section at the autoionization thresholds, we have assumed that the probability of decay into the continuum is unity, when the electron is excited to an autoionizing level.

3. Results and discussion

Electron impact ionization cross-sections for Ba have been plotted as a function of the incident energy in figure 1. The figure includes, in addition to the present cross-sections

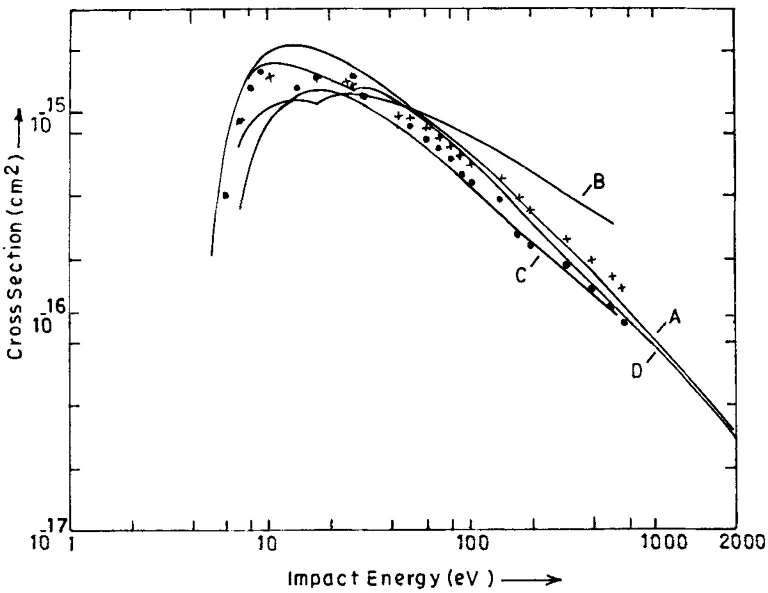

Figure 1. Electron impact ionization cross-sections for Ba; (**A**) Present calculation including contributions from inner shells and excitation-autoionization; (**B**) Calculation of Lotz [17]; (**C**) Calculation of McGuire [18]; (**D**) Present calculation (including contributions from inner shells) excluding excitation-autoionization. (●) Experiment of Dettmann and Karstensen [19]; (×) Experiment of Okudaira [20]

(including and excluding contributions from excitation autoionization), the theoretical results of Lotz [17] and McGuire [18] and experimental observations of Dettmann and Karstensen [19] and Okudaira [20]. We have used the transition $5p^6s^2$—$5p^5 6s^2 5d^1$ occurring at the energies 12·0–15·0 eV to calculate the excitation-autoionization cross-sections. Our direct calculation of ionization cross-sections incorporates the contribution from the inner shells 5p, 5s and 4d. The calculated cross-sections (including contributions of excitation-autoionization) are always within a factor 2 of the experimental observations at all impact energies. It is observed that the indirect process i.e. excitation-autoionization, significantly enhances the cross-sections near excitation threshold and our cross-sections slightly overestimate the experimental value. The first peak which can be attributed to the excitation-autoionization appears at near 100 eV in both the experiments, whereas the corresponding peak appears at 120 eV in our calculations. Our cross-sections are in better agreement with both the experiments below the energy range 100 eV than those of Lotz [17] and McGuire [18]. In the energy region above 100 eV, our cross-sections correspond well with the experimental observations of Okudaira [20] whereas McGuire's results are in closer agreement with the experimental observations of Detmann and Karstensen [19].

The calculated and experimental cross sections for Ba^+ have been shown in the figure 2. For comparison with other theory, we have also plotted the only theoretical results of Bely *et al* [21]. Transitions $5p^5 5d(^3p)6s^2 p_{1/2,3/2}$–$5p^5 5d(^1p)^2 p_{1/2,3/2}$ [22a, b] appearing at the energies 15·96 eV and 21·05 eV, respectively, have been used to calculate the excitation-autoionization cross-sections. Our calculated cross-sections are always within a factor 2 of the experimental observations of Peart and Dolder [23] and Feeny

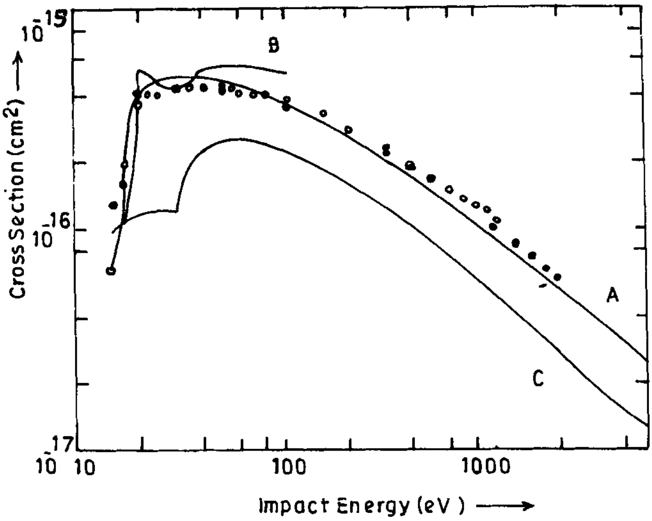

Figure 2. Electron impact ionization cross-sections for Ba^+; (A) Present calculation including contributions from inner shells and excitation-autoionization; (B) Calculation of Bely *et al* [21]; (C) Present calculation (including contributions from inner shells) excluding excitation-autoionization. (●) Experiment of Peart and Dolder [23]; (○) Experiment of Freney *et al* [24]

et al [24] throughout the energy range investigated except at excitation-autoionization threshold. The peak (at 20 eV) due to excitation-autoionization in our calculation corresponds well the experimental peak in both the experiments. The present cross-sections are in better agreement with experiments than those of Bely *et al* [21] in the energy range 20–100 eV, whereas the results of Bely *et al* [21] are close to the experiments below 20 eV. As there is no other theoretical work in the energy range larger than 100 eV, we are unable to compare our results with others. In this energy range, our cross-sections are in excellent agreement with both the experiments.

Theoretical as well as experimental cross-sections for Ba^{2+} have been shown in figure 3 and we have used the transitions $5s^2 5p^6 - 5s5p^6 nl - 5s^2 5p^5 + e$ and $4d^{10} 5s^2 5p^6 - 4d^9 5p^6 4f$ appearing at energies 40·9 eV–42·1 eV and 90·7 eV–118·0 eV, respectively, to calculate the excitation-autoionization cross-sections. Our calculated cross sections are always within a factor 2 of the experimental observations of Tinschert *et al* [3] throughout the energy range investigated except below the excitation-autoionization threshold. The peak corresponding to excitation-autoionization shifts left on the energy axis. This may be attributed to the fact that the hydrogenic velocity distribution of the bound electrons for Ba^{2+} has been used. As the Hartree–Fock velocity distribution reduces the cross-section in low energy range and enhances in high energy range compared to the hydrogenic velocity distribution, the use of HF velocity distribution may improve our calculation both in lower and higher energy ranges. In high energy range, our results underestimate the experiments. Plane wave (PW) calculations [3] available in the energy range 40–200 eV are certainly in better agreement with experiments than the present ones.

It is observed that the direct total ionization cross-section decreases appreciably with increase in the charge state of the target atom (ion). On the other hand the excitation-autoionization cross-section increases significantly with increase in the charge state.

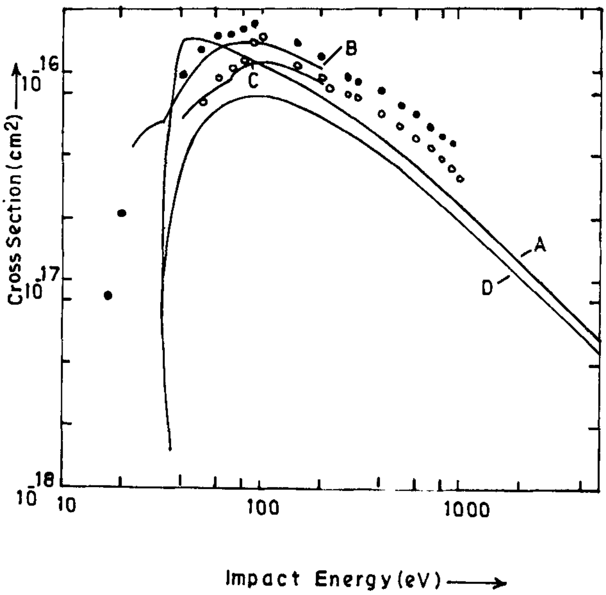

Figure 3. Electron impact ionization cross-sections for Ba^{2+}; (**A**) Present calculation including contributions from inner shells and excitation-autoionization; (**B**) D W calculation for direct ionization of 5p and 5s in metastable state [3]; (**C**) D W calculation for direct ionization of 5p and 5s in ground state [3]; (**D**) Present calculation (including contributions from inner shells) excluding excitation-autoionization; (●) Experiment of Tinschert *et al* [3] employing Penning ion-source; (○) Experiment of Tinschert *et al* [3] employing hot ECR ion source.

The decrease in the total ionization cross-section with increase in charge state can be understood in terms of the fact that the binding energies for the shells of the atom (ions) increase remarkably with increase in charge state. The same fact is probably responsible for the increasing excitation-autoionization cross-sections with increase in charge state of atom (ion) which we have observed in our calculations. In the case of greater charge state of target ion, the binding energies of inner shells are larger and the electron getting excitation there from may go into the autoionization level well above the first ionization limit [see 25 and references therein]. This leads to greater probability to decay into the continuum. The overestimation near excitation-autoionization threshold is a general feature [see 5 and references therein]. However, the overestimation can be reduced to some extent by multiplying the excitation cross-section by the branching ratio $(A_a/A_a + A_r)$, A_a and A_r being the transition probabilities for autoionization and radiative decay, respectively.

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