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Electron impact ionization of Zn^+ and Ga^+

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Abstract. We have investigated the contribution of excitation-autoionization to the electron impact ionization of Zn^+ and Ga^+ using the binary encounter approximation. Hartree-Fock velocity distributions for the bound electrons have been used throughout the calculations of direct and indirect ionization cross-sections. The calculated cross-sections are in good agreement with recent experiments. We have also compared our results with other theoretical calculations.

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

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1. Introduction

Various theoretical and experimental investigations have admittedly considered the importance of indirect ionization processes to the electron impact ionization of positive ions. Excitation-autoionization and resonant excitation double autoionization (REDA) processes are the important indirect physical mechanism for ionization which received considerable theoretical and experimental attention in recent years [1]. In the excitation-autoionization process, 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 [2–7]. Accurate knowledge of electron impact cross-sections is necessary for an understanding of ionization equilibrium or ion abundance in astrophysical and laboratory plasmas. Zn^+ and Ga^+ are, respectively, Cu-like and Zn-like structures. These particular ions are not normally found in plasmas, but heavier species stripped to these configurations may be present in tokamaks in high enough abundance to be important in determining the energy balance via line radiation.

As far as the theoretical aspect of electron impact ionization of these ions (Zn^+ and Ga^+) is concerned, scaled PWB cross-sections of McGuire [8] and Lotz cross-sections [9, 10] based on semiempirical formula are available in literature. In Zn^+, Rogers *et al* [11] calculated excitation-autoionization cross-section in two state close coupling and added it to the scaled PWB cross-section. In a similar way, Pindzola *et al* [12] also calculated excitation-autoionization cross-section for Ga^+ in distorted wave approximation and added it to the scaled PWB cross-section. Crandall [2] pointed out that the scaled PWB is appropriate for neutral atoms but is less appropriate for ions. Lotz formula is not physically sound, and is limited to incorporate the excitation-autoionization process. On the other hand, the binary encounter (BE) description of excitation-autoionization contributing to the electron impact ionization has been found satisfactorily agreeing with experiments, especially in heavier ions [13, 14]. Keeping in view the limitations of scaled PWB cross-sections in positive ions and satisfactory agreement of BEA with experiments, we consider it worthwhile to investigate theoretically the electron impact ionization of Zn^+ and Ga^+ including excitation-autoionization in BEA.

In the present work, Vriens [15] 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 has been incorporated along the line suggested by Thomas and Garcia [16] (see also [17, 13]).

2. Theoretical consideration

Vriens expressions incorporating the effect of Coulomb deflection for electron impact ionization and excitation cross-sections can be written in terms of dimensionless variables [13, 14],

$$Q_{\mathrm{I}}(s,t)=\frac{(s+s')^2}{s^2(s'^2+t^2+1)}\left[\frac{s'^2-1}{U^2s'^2}+\frac{2t^2}{3}\left(\frac{s'^4-1}{U^2s'^4}\right)-\frac{\phi'}{U^2(s'^2+1)}\ln s'^2\right](\pi a_0^2) \tag{1}$$

and,

$$\begin{aligned}Q_{\mathrm{E}}(s,t)=&\frac{(s+s')^2}{s^2(s'^2+t^2+1)}\left[\frac{1}{U}\left(\frac{1}{U_n}-\frac{1}{U_{n+1}}\right)+\frac{2}{3}t^2\left(\frac{1}{U_n^2}-\frac{1}{U_{n+1}^2}\right)\right.\\&+\frac{1}{U}\left(\frac{1}{s'^2U+U-U_{n+1}}-\frac{1}{s'^2U+U-U_n}\right)\\&+\frac{2}{3}t^2\left(\frac{1}{(s'^2U+U-U_{n+1})^2}-\frac{1}{(s'^2U+U-U_n)^2}\right)\\&\left.-\frac{\phi''}{(s'^2+1)U}\ln\left(\frac{U_{n+1}(s'^2U+U-U_n)}{U_n(s'^2U+U-U_{n+1})}\right)\right](\pi a_0^2),\ s'^2U>U_{n+1}\\=&\frac{(s+s')^2}{s^2(s'^2+t^2+1)}\left[\frac{1}{U}\left(\frac{1}{U_n}-\frac{1}{s'^2U}\right)+\frac{2}{3}t^2\left(\frac{1}{U_n^2}-\frac{1}{(s'^2U)^2}\right)\right.\\&+\frac{1}{U}\left(\frac{1}{U}-\frac{1}{s'^2U+U-U_n}\right)+\frac{2}{3}t^2\left(\frac{1}{U^2}-\frac{1}{(s'^2U+U-U_n)^2}\right)\\&\left.-\frac{\phi''}{(s'^2+1)U}\ln\left(\frac{s'^2(s'^2U+U-U_n)}{U_n}\right)\right](\pi a_0^2),\\&U_n\leqslant s'^2U\leqslant U_{n+1}.\end{aligned} \tag{2}$$

The expressions for ionization and excitation cross-sections have been integrated over the Hartree-Fock velocity distribution for the bound electrons. Hartree-Fock radial functions given by Clementi and Roetti [18] have been used to construct the momentum distribution function. 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

The calculated electron impact ionization cross-sections for Zn^+ along with the experimental observations of Rogers *et al* [11] and of Peart *et al* [19] have been presented in figures 1 and 2. For comparison, we have plotted the only competent quantal calculation of Rogers *et al* [11] who have calculated the close coupling excitation autoionization cross-sections and added to the scaled PWB cross-sections [8]. The scaled PWB and Lotz cross-sections have also been shown in these figures, although these do not include the contribution of excitation-autoionization. We have taken the contributions of direct ionization from the inner shells $3d$, $3p$ and $3s$ to the direct ionization of the valence $4s$ electron. The calculated total cross-sections also include the contribution of the indirect process of excitation-autoionization. We have taken the transitions $3d^{10}4s-3d^94s(^1D)5p(^2P^0)$ and $3d^{10}4s-3d^94s(^3D)5p(^2P^0)$ reported by Rogers *et al* [11] to calculate excitation-autoionization cross-sections. Our cross-sections are within the factor 1·5 of the experimental observations at all impact energies larger than 22 eV. The first peak corresponding to the excitation-autoionization appears at 26 eV in our calculation. There is no clear indication of such peaks in both experiments, but slight variation in cross-section in the experiments can be seen at the same impact energy. The second peak corresponding to the contribution of the inner shell $3d$ appears at 53 eV whereas the same peak is observed at 60 eV in the experiment of Rogers *et al.* However, the magnitude of these peaks differ slightly. The slight hump in both theoretical and experimental cross-sections at 120 eV is due to the inclusion of ionization from inner shell $3p$. The present results are in better agreement with experiments than the calculations of Rogers *et al* (excitation-autoionization + scaled PWB) in the energy range up to 50 eV. In the energy range between 50 eV and 100 eV, the cross-sections of Rogers *et al* are close

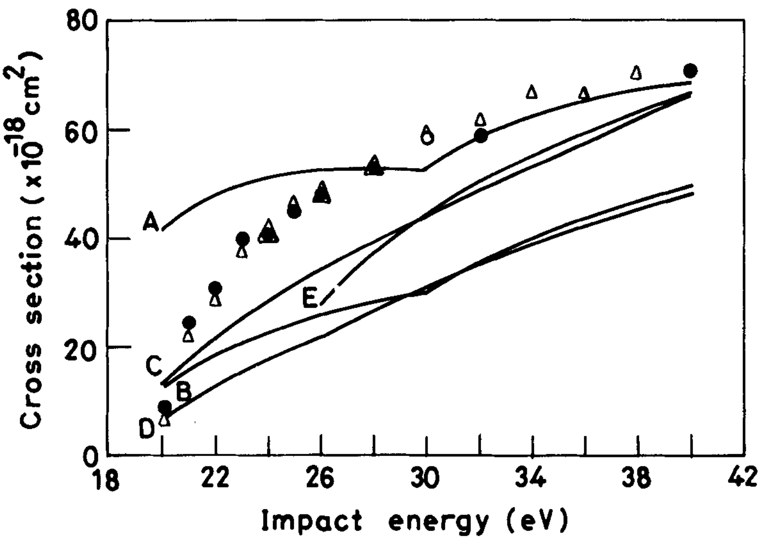

Figure 1. Electron impact ionization cross-sections for Zn^+; A. Present calculation including contributions from inner shells and excitation-autoionization; B. Present calculation (including contributions from inner shells) excluding excitation-autoionization; C. Calculation of Lotz [9]; D. Scaled PWB calculation of McGuire [8]; E. Excitation-autoionization + Scale PWB calculation of Rogers *et al* [11]; Δ Experiment of Peart *et al* [19]; ● Experiment of Rogers *et al* [11].

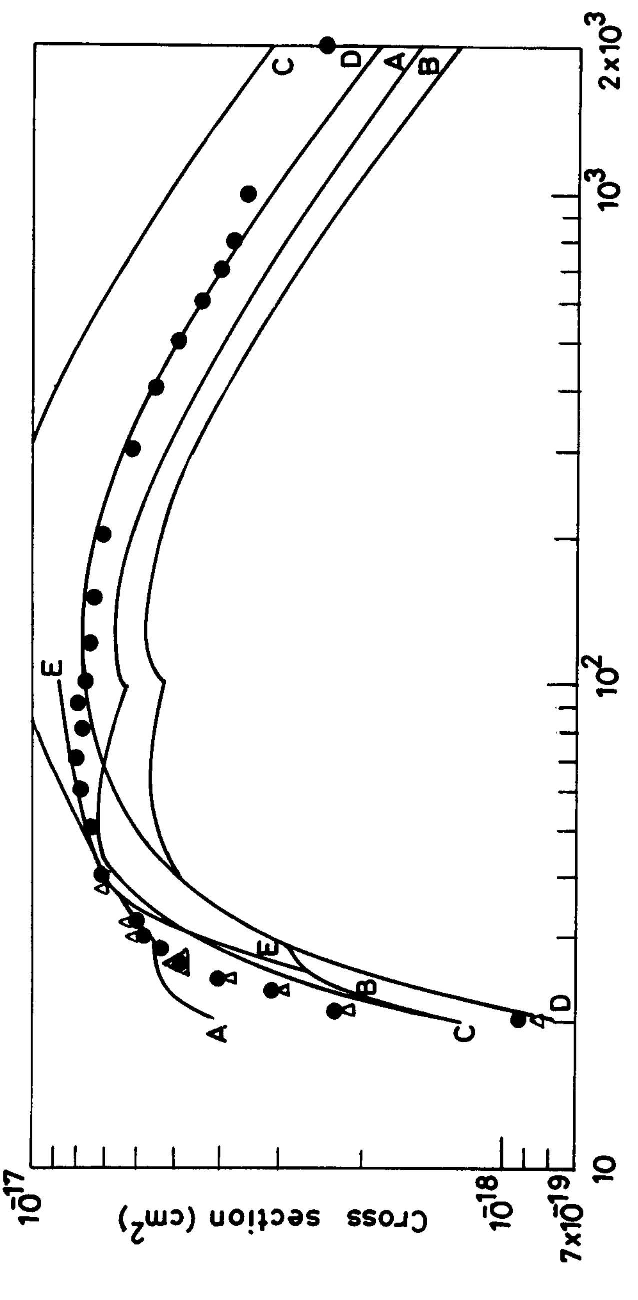

Figure 2. Electron impact ionization cross-section for Zn^+; Explanation for the curves is the same as that given for figure 1.

to the experiment compared to the present one. Beyond 100 eV, it is difficult to draw any definite conclusion about the agreement of the theoretical results of Rogers *et al* with experiments, as their calculations are limited up to 100 eV only. The scaled PWB cross-sections which do not include the contribution of excitation-autoionization are close to the experiment as compared to our cross-sections beyond 70 eV whereas the present calculation is in better agreement with the experiments below 70 eV. The semiempirically calculated cross-sections of Lotz are close to the experiment at energies up to 25 eV as compared to the present calculation. Beyond 25 eV, the present results agree well with experiments whereas Lotz's calculation tends to overestimate the experimental cross-sections. No hump or specific peak has been noticed in these quantal or semiempirical calculations.

In Ga^+ (figures 3 and 4) we have taken the contributions of direct ionization from the inner shells $3d$, $3p$ and $3s$ to the direct ionization of $4s$ valence electron. The transitions $3d^{10}4s^2 - 3d^9 4s^2 4p(^3P_1, {}^1P_1, {}^3D_1)$ reported by Pindzola *et al* [12] and suggested by Peart and Underwood [20] have been used to calculate the excitation-autoionization cross-sections. Our calculated cross-sections are always within a factor 1·5 of the experimental values throughout the energy range investigated except at excitation-autoionization threshold where the largest factor is 2. Our first peak corresponding to the excitation-autoionization appears at 32 eV. There is no obvious indication of such peak in the experiment of Rogers *et al* [11]. However, a slight variation in the cross-sections of Peart and Underwood [20] can be seen at the same impact energy. The second peak which corresponds to the direct ionization from the inner shell $3d$ appears at 40 eV which is consistent with the experiments. In lower energy range (up to 100 eV), our calculated cross-sections are in better agreement with both the experiments than scaled PWB and Lotz cross-sections. Beyond 100 eV

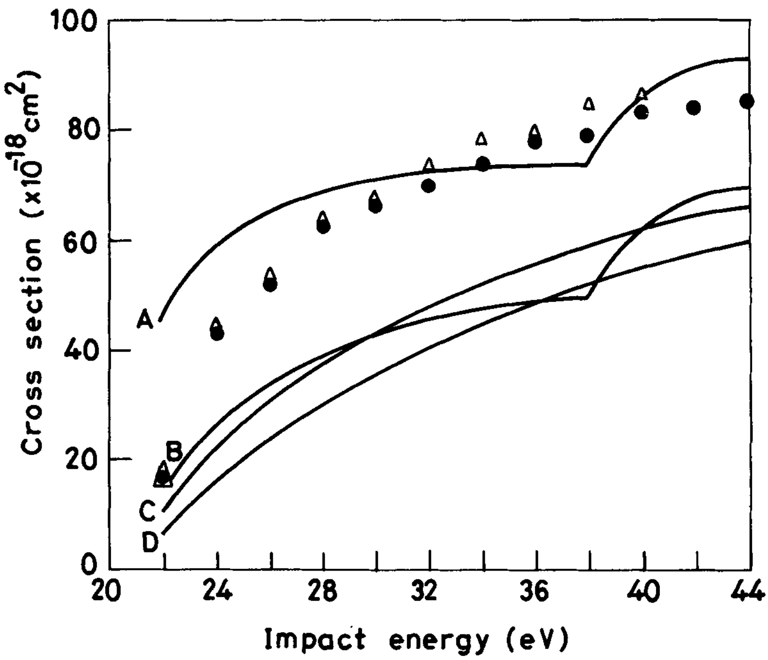

Figure 3. Electron impact ionization cross-sections for Ga^+; Explanation for the curves is the same as that given for figure 1. Δ, Experiment of Peart and Underwood [20].

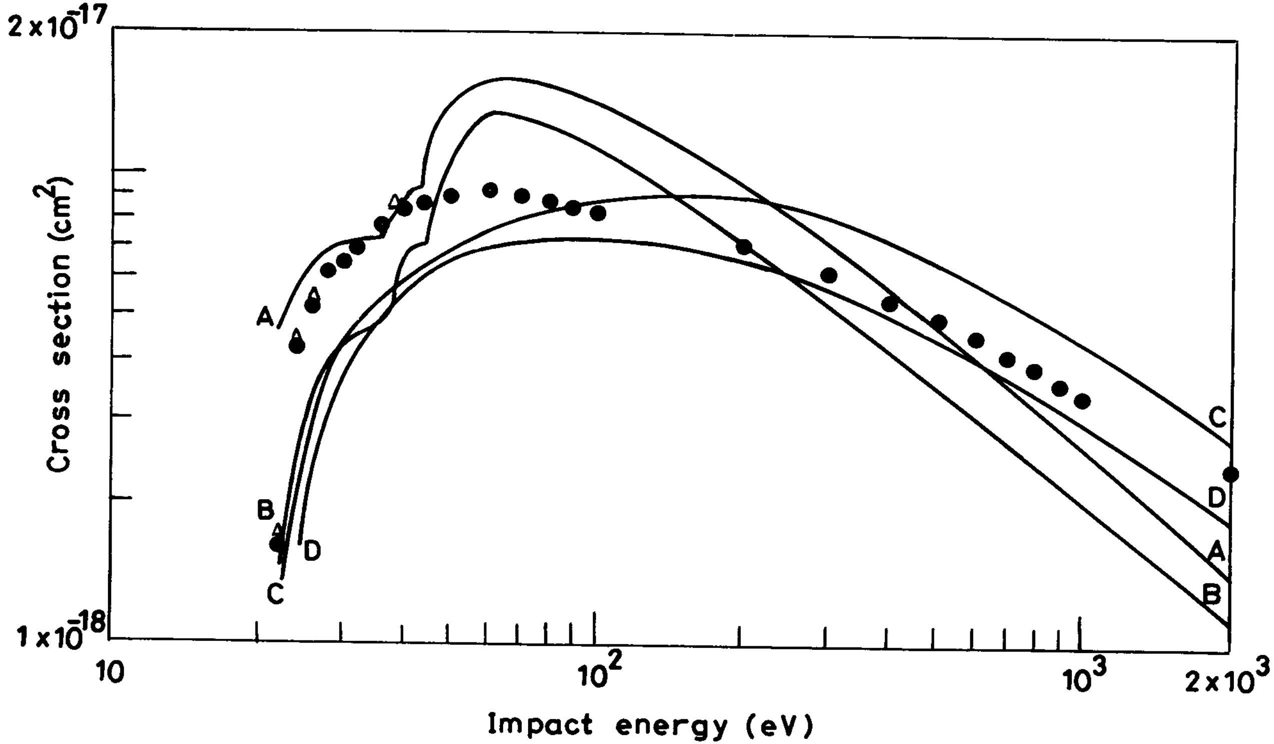

Figure 4. Electron impact ionization cross-sections for Ga^+; Explanation for the curves is the same as that given for figure 1. Δ, Experiment of Peart and Underwood [20].

scaled PWB and our calculations are identically agreeing with the experimental observations of Rogers *et al* [11] whereas Lotz calculations overestimate the cross-sections. No other suitable quantal calculation including excitation-autoionization is available for the comparison with our results.

In figures 1–4, our calculated cross-sections overestimate the experimental observations near excitation-autoionization threshold by 2. The overestimation of the present results in the low energy region can be attributed to the non-suitability of the BEA. The overestimation near excitation-autoionization threshold may be partly due to the fact that we have taken non-radiative decay probability to be unity. This overestimation is a general feature [2, 11, 14] and it may be reduced to some extent by multiplying the excitation cross-sections by the branching ratio $A_a/(A_r + A_a)$, A_a and A_r being the transition probabilities for autoionization and radiative decay, respectively [13]. Keeping the above discussions in view, we conclude that the BEA gives reasonably satisfactory agreement with experiments despite its limitations in explaining excitation process more correctly.

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