

INFLUENCE OF SUBVALENCE nd^{10} SHELL ON THE EXCITATION
OF RESONANCE LINES OF Al^+ SUBGROUP IONS

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Abstract. The results of comparative analysis of energy dependences of effective cross-sections for electron-impact excitation of resonance $nsnp\ ^1P_1 \rightarrow ns^2\ ^1S_0$ transitions in ions of Al^+ subgroup are presented. The values of excitation cross-sections for the Ga^+ , In^+ and Tl^+ ion resonance lines are found to be comparable in the entire energy range under investigation. The increase of the atomic number of an ion is shown to result in the increase of contribution of the resonance processes into the effective electron-impact excitation cross-sections for resonance line due to the increasing role of relativistic and correlation effects. Correlations not only within closed s^2 and d^{10} shells, but also between them are shown to be significant.

1. INTRODUCTION

Data for the electron-impact excitation of positive ions are necessary to model and diagnose high-temperature plasmas important in controlled-fusion research and astrophysics. Single- and multiply-charged ions occur in these environments and it is important to have knowledge of collision cross sections for the analysis and diagnostics of such plasmas. Most of the existing data for electron-impact excitation of positive ions come from theoretical calculations. Experimental measurements are needed to provide tests of the theoretical methods.

A first stage of beam studies has resulted in the elucidation of the general regularities of electron scattering by ions and in the determination of effective cross sections, primarily for light single-charged ions. The development of experimental techniques in recent years has rendered the detailed study of scattering cross sections of electrons by heavy ions and particularly their resonance structure increasingly practicable. This structure is caused by the dielectronic capture of the incident electron by the excited-ion target into a short-lived autoionizing states (AIS) followed by autoionization to an excited state (resonance excitation). However, heavy many-electron ions have not been studied nearly as much, and discrepancies are found between experimental measurements and various predictions.

Despite the active experimental investigations in different scientific teams worldwide, that began with the first precise experiments using crossed beams, as well as the sound theoretical work on the resonance account, reliable data on electron

collisions with ions have been obtained only for a limited number of ionic targets. With limited data, a comprehensive, systematic and consistent interpretation of electron-ion scattering mechanisms has yet to be achieved – and can only be realized by in-depth studies involving electron correlation effects.

Our recent investigations of Zn^+ (see, e.g. Imre *et al.* 2000) and Cd^+ (see, e.g. Gomonai 2003) ions with filled subvalent nd^{10} shell show that in this case the resonance processes are substantially complicated due to the intershell interaction and relativistic effects. Up to now these and another new high-order effects are not fully explained. In this connection, the studies of the excitation processes in the collisions of slow electrons with ions of Al^+ subgroup seem to be of a particular interest.

In this paper, we report on the results of comparative analysis of the experimental resonance line electron-impact excitation cross-sections for In^+ ion investigated by our group (Gomonai *et al.* 2005), Ga^+ (Stefani *et al.* 1982) and Tl^+ (Imre *et al.* 1989) ions. These ions are the heaviest homologue in the group *II-B* alkaline-earth Zn -, Cd - and Hg -like systems, which have the $(n-1)d^{10}ns^2$ ground configurations.

2. EXPERIMENTAL APPARATUS AND PROCEDURE

The measurements were performed using a crossed-beam technique with an apparatus previously described elsewhere (Gomonai 2003). The experiment including metal indium is a complicated and laborious task for a number of reasons: (*i*) desired indium atom vapor pressure in the ion source ($10^{-3} - 10^{-2}$ Torr) is reached at high temperatures (900–1000) °C, while indium melting point is 156 °C; (*ii*) at such temperatures this metal is chemically aggressive that results in the destruction of ion source parts and intense production of liquid metal phase at the ceramic insulators; (*iii*) when the ion source operates in the discharge mode, the low-lying metastable $^3P_{0,2}^o$ -states of In^+ ion could be produced effectively. The above peculiarities put strict requirements on the ion source design. We have developed new design of the ion source (Gomonai *et al.* 2005), which allowed one to take into account these requirements and obtain a stabilized In^+ ion beam ($E_i = 700$ eV, $I_i = 2 \times 10^{-6}$ A). Electron beam current in the energy region of $E_e = (7-300)$ eV was $I_e = (7-30) \times 10^{-5}$ A at the energy spread (FWHM) of $\Delta E_{1/2} = 0.4$ eV. Spectral separation of radiation was carried out by means of a vacuum monochromator based on the Seya-Namioka scheme. The inverse linear dispersion of monochromator was $d\lambda/dl = 1.7$ nm/mm. A cooled solar-blind photomultiplier was used to detect radiation. Modulation of both beams by square voltage pulses phase-shifted by 1/4 of the modulation period was used to extract the signal due to the process under study against the total background. The signal of the $(1 - 0.2)$ s^{-1} magnitude was extracted against the background at the signal to background ratio 1/10 to 1/30. The process of the measurements and analysis of results were automated using an IBM PC. The electron energy scale was calibrated with the 0.1 eV accuracy.

3. RESULTS AND DISCUSSION

The results of the Ga^+ , In^+ and Tl^+ ($nsnp\ ^1P_1^o \rightarrow ns^2\ ^1S_0$) resonance line emission cross-section measurements are shown in Fig. 1. The energy dependences of the cross-sections behavior at threshold are consistent with an infinitely steep rise folded with

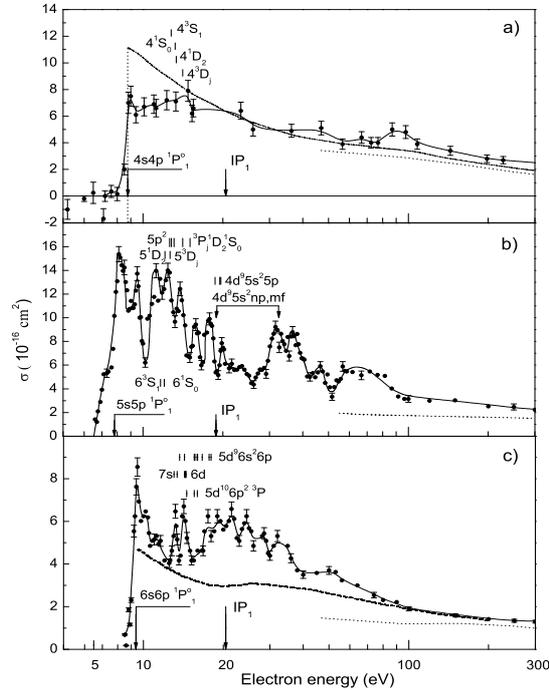


Figure 1: Electron excitation functions for the resonance lines: a) Ga^+ ion; b) In^+ ion; c) Tl^+ ion (dots - experiment data; dotted lines - calculation by Van-Regemorter formula; chain line - calculation by the g-factor formula; long dotted line - close-coupling approximation).

the 0.6 eV (Ga^+), 0.4 eV (In^+) and 0.5 eV (Tl^+) energy spread of the electron beam. Above 100 eV the data fall off with the predicted $\ln E/E$ energy dependence.

The absolute value of the emission excitation cross-sections for the resonance $\lambda = 158.6$ nm line of In^+ ion was obtained by normalizing the experimental excitation functions to the semi-empirical calculation by the Van-Regemorter formula at the 300 eV electron energy (see Fig. 1b, dotted curve). The uncertainty of the absolute effective excitation cross-section determination was about 30 percent.

The absolute cross-section for Ga^+ ion resonance line was obtained by normalizing the excitation function to the experimentally determined absolute excitation cross-section standard at the energy 6.9 ± 0.5 eV ($\sigma = (5.0 \pm 0.6) \times 10^{-16} \text{ cm}^2$) (Stefani et al. 1982) and for Tl^+ ion – by normalizing to the theoretical calculation at the 100 eV energy using the close-coupling method taking into account two stages ($\sigma = (1.9 \pm 0.8) \times 10^{-16} \text{ cm}^2$) (Imre et al. 1989).

As seen from Fig. 1, the excitation cross-section values for the Ga^+ , In^+ and Tl^+ ion resonance lines are comparable in the entire energy range under study, and the maximum of the effective excitation cross-sections was observed for In^+ ion, that, probably, can be explained by the lowest value of the $5s5p \ ^1P_1^o$ resonance level

excitation energy. Peculiarities revealed in the excitation functions result from both the resonance contribution due to formation and decay of short-lived AIS of *Ga* (Dunn et al. 1993), *In* (Bhatia 1978), *Tl* (Baig et al. 1992) atoms and cascade transitions from higher ion levels. As seen from Fig. 1a, the contribution of these processes is the smallest for the Ga^+ ion resonance line effective cross-section. In our opinion, this is due to the fact that for this ion, as the lightest one ($Z = 31$), the resonance contribution can result only due to correlation effects inside the valence s^2 closed shell. In this case, the influence of the subvalence d^{10} shell is not determinative because, as the estimative calculations of the average radii of the valence and subvalence shells of Ga^+ ion using Hartree-Dirac formula show, the above shells are located at large distances from each other.

For a heavier In^+ ion ($Z = 49$), the peculiarities in the energy dependence of the effective electron-impact excitation cross section for the resonance line are, first of all, due to the resonance processes with the essential role being played by correlation effects both inside the valence s^2 shell (as observed below 12 eV) and between the valence s^2 and subvalence shells (above 12 eV) due to the close electron binding energies in these shells.

For the heaviest Tl^+ ion ($Z = 81$) the effect of configuration interaction is larger, and correlation and relativistic effects are more essential. In this ion, the presence of the $4f^{14}$ shell in the total configuration of the electron core results in a strong screening of the Tl^+ ion nucleus. As a result, the electron trajectories in the valence and subvalence shells overlap (their average radii differ less than twice). As shown in (Deselaux and Yong-Ki Kim 1975), the binding energies of the $6s^2$ -electrons increase to 30 percent and for the $5d^{10}$ -electrons decrease to 15 percent as compared to non-relativistic case, i.e. the role of the $5d^{10}$ shell in the excitation process significantly increases. In case of Tl^+ ion the AIS formed at the excitation of one of the $5d^{10}$ -electrons are located lower and they are an important channel of the resonant contribution to the excitation of these ionic resonance levels.

Resonance phenomena strongly affect all collision processes and can considerably influence their cross sections, especially in the near-threshold region. The resonance contributions dominate over the direct scattering in this energy region and strongly depend on Z . The mechanisms of both direct and resonance collision processes are considerably complicated by the relativistic and correlation effects, which are extremely essential in the complex multielectron systems characterized by effectively excited nd- subvalence shell.

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