Classical treatment of Li$^{2+}$+Ar and He$^{2+}$+Ar collisions

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Synopsis: Classical Trajectory Monte Carlo calculations are carried out for Li$^{2+}$+Ar and He$^{2+}$+Ar collisions, motivated by recent experiments on these systems. Cross sections for electron capture, projectile electron loss and target multiple ionization processes are evaluated and compared to the experimental values in the 75-500 keV/amu impact energy range.

Absolute cross sections for electron capture and projectile electron loss, eventually accompanied by target ionization, have been measured recently in Li$^{2+}$+Ar collisions in the 75-500 keV/amu impact energy range [1]. We therefore performed calculations of these cross sections, in the framework of the impact-parameter Classical Trajectory Monte Carlo (CTMC) method [2]. Our calculations employ a two-active electron description, with one active electron on both target and projectile centres, in order to address dynamical processes involving both target and projectile electrons [3]. The interaction of these active electrons with the frozen target ionic core Ar$^+$ is described by means of a (mean-field) model potential, similar to what was performed in [4]. High-order processes, as target multiple ionization, are evaluated within the Independent Particle Model (IPM, [5]), where the multi-electron probabilities are obtained as products of one-electron probabilities.

The comparison of computed and measured cross sections enables to gauge the accuracy of the IPM and underlying model potential descriptions. We illustrate this in Figure 1 where are displayed the cross sections for multiple ionization of Ar accompanied by single electron loss of Li$^{2+}$. The agreement between theory and experiment is satisfactory, which signs the adequacy of the IPM to calculate high-order cross sections and of the classical collisional treatment to compute the underlying one-electron probabilities, from intermediate to high impact velocities.

As stated in [1], cross sections for Li$^{2+}$+Ar collisions can interestingly be compared to those for He$^{2+}$+Ar collisions [6], in order to assess the influence of projectile ionic cores on the dynamical processes. In the case of He$^{2+}$ impact, we employed, alternatively to CTMC, a semi-classical monocentric approach [7] to obtain the one-electron probabilities entering the IPM. These probabilities are in good agreement with their classical counterparts, and the projectile ionic core is generally found to be of little importance in the impact energy range considered.

Details on the calculations and extensive comparison of theoretical and experimental results will be presented at the Conference.

Figure 1. Cross sections for Li$^{2+}$+Ar $\rightarrow$ Li$^{3+}$+Ar$^{j+}$+(j+1)e. Symbols: experiments [1]; lines: present calculations.

References


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