B-spline R-matrix with pseudo-states calculations for electron-impact ionization plus excitation of magnesium

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Synopsis The B-spline R-matrix with Pseudo-States method is employed to treat electron-impact ionization of magnesium atoms. The present non-perturbative calculations cannot resolve the significant differences between experiment and theory for the ionization-excitation processes. Instead, they confirm the relative normalization from previous calculations.

In recent years, much progress has been made in the theoretical and computational treatment of direct electron impact ionization processes. (See [1] for a recent review.) The situation, however, does not look as good for the more complex process of ionization with excitation. Although satisfactory results were obtained for He [2], similar studies for Mg [3] show that the ratio of the triple-differential cross section (TDCS) for ionization with excitation to the three lowest excited states of Mg^+ to that for ionization without excitation might have been predicted by factors of 2–20 smaller by theory than what was determined experimentally [4].

The purpose of the present work was to carry out independent calculations to either resolve or shed more light on these significant differences between experiment and theory. Based on the successful description of the ionization-excitation process for He [2], we expect a similar accuracy for Mg, which is also treated as a quasi-two-electron system. In the present work, the B-spline R-matrix method [2] was used to study electron collisions with neutral magnesium over an energy range from threshold to 400 eV. The scattering model included 712 coupled states, most of which were continuum pseudo-states that simulate the true ionization continuum of the target up to 50 eV. We obtained good agreement with existing experimental data for the total ionizations cross sections over a wide range of incident electron energies. This indicates the completeness of the pseudo-state basis employed in our work.

Our calculations also suggest a relatively large contribution of the ionization plus excitation processes. In Figure 1, the experimental TDCS results [4] are compared with predictions from the DWB-RM model (also shown in [4]) and the present BSR calculations. Note that the theoretical values were renormalized with the factors indicated for a good visual agreement with experiment. We see quite satisfactory agreement in shape between experiment and theory. However, even though the theoretical predictions exhibit some model dependence, especially for the larger ejected-electron angles, we cannot resolve the significant differences between experiment and theory in the absolute values.

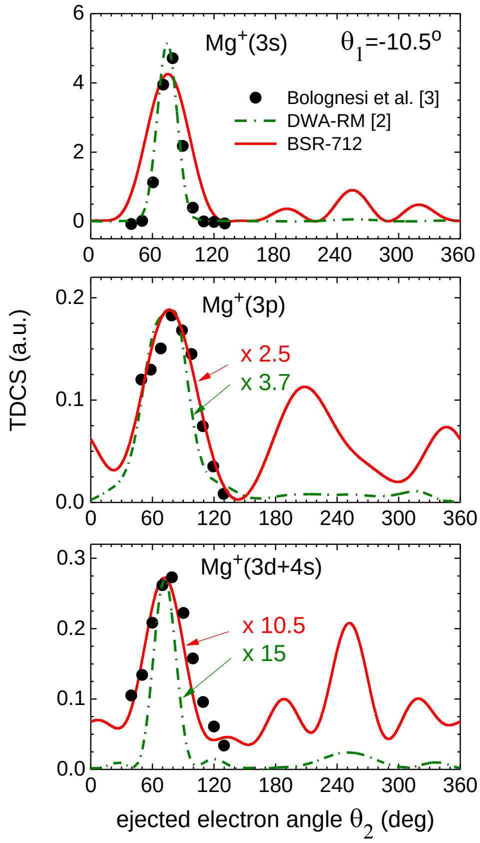

Figure 1. TDCS for the Mg^+ 3s, 3p and 4s+3d final ionic states measured at E_1 = 400 eV, E_2= 20 eV and θ_1 =10.5°. The experimental results (solid circles) are compared with predictions from the DWB-RM [4] (dash-dotted line) and BSR (solid line) calculations.

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References

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