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

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Synopsis The B-spline R-matrix with pseudo-states method was employed to treat electron collisions with magnesium atoms. Predictions for elastic scattering, excitation, and ionization (including ionization plus excitation) were obtained for all transitions between the lowest 25 states of magnesium. The accuracy of the predictions was checked by comparing with available experimental data and with results obtained in different approximations with increasing number of coupled states.

Electron scattering from magnesium has been intensively studied both experimentally and theoretically. Most previous calculations, however, were devoted to selected individual transitions and a few energies (see [1] for references). The purpose of the present work, therefore, is to provide a comprehensive set of results that covers essentially all recent experimental data. This systematic comparison of available experimental and theoretical results makes it possible to assess the accuracy of the existing data and to search for possible sources of the main discrepancies between experiment and theory.

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 100 eV. The largest scattering model included 712 coupled states, most of which were pseudo-states that simulate the effect of the high-lying Rydberg continuum and, most importantly, the ionization continuum on the results for transitions between the discrete states of interest. This effect is particularly strong at "intermediate" incident energies of a few times the ionization threshold.

As an example, Fig. 1 shows the $(3s3p)^1P^o$ excitation. The differences between the BSR-37 and BSR-712 results illustrate the influence of the target continuum. Our most extended BSR-712 cross sections are in close agreement with recent CCC results [3]. This indicates the likely convergence of both calculations. At the same time there is a noticeable difference with the experimental measurements [4] at lower energies. This calls for further checking the absolute normalization in [4], in particular since these data are used for the normalization of cross sections for other transitions [5] and hence may severely affect their accuracy.

Figure 2 shows ionization cross sections, including ionization plus excitations. We see relatively large contributions from the latter processes. The good agreement with existing experimental data over a wide range of incident electron energies indicates the completeness of the pseudo-state basis and can be considered as an additional confirmation of the accuracy of the entire data set.

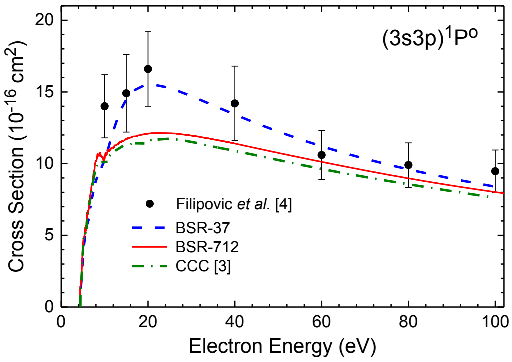

Figure 1. Electron-impact excitation cross sections of the $(3s3p)^1P^o$ resonance transition in Mg.

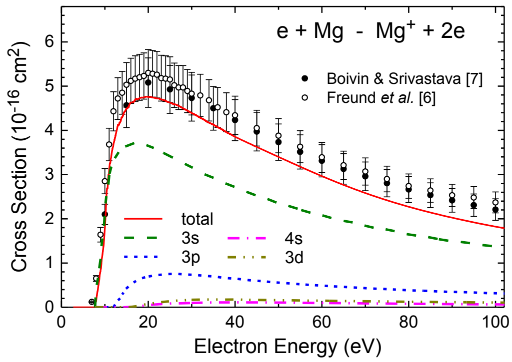

Figure 2. Electron-impact ionization cross sections for neutral Mg in different final ionic states.

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References

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