Electron excitation of the $3s4s\ ^1S_0$ and $3s4p\ ^1P_1$ states of magnesium

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(Received 5 May 2008; published 10 July 2008)

Prompted by the recent measurements of Predojević *et al.*, we have calculated the excitation of the $3s4s\ ^1S_0$ and $3s4p\ ^1P_1$ states of magnesium by electron impact at 20, 40, 60, and 100 eV in the relativistic distorted-wave approximation. Results are presented for the differential and integrated cross sections and compared with previous experimental and theoretical data.

DOI: 10.1103/PhysRevA.78.014701 PACS number(s): 34.80.Dp

Predojević *et al.* [1] have recently measured the differential cross sections (DCSs) for the electron impact excitation of the $3s3d\ ^1D_2$, $3s4s\ ^1S_0$, and $3s4p\ ^1P_1$ states of magnesium from the ground $3s^2\ ^1S_0$ state. This is a continuation of earlier work on the excitation of the $3s3p\ ^1P_1$ state [2,3] which reported combined experimental measurements and new theoretical relativistic distorted-wave (RDW) calculations. We have previously carried out RDW calculations for the excitation of the various fine-structure levels of the $3s3p$ and $3s3d$ configurations using simple spectroscopic-configuration wave functions to represent the initial and final states [4]. The results for the $3s3d$ configurations were later refined by using more elaborate multiconfiguration wave functions [5]. Predojević *et al.* [1] compared their measured DCS results for the $3s3d\ ^1D_2$ state with these latter calculations as well as the earlier measurements of Williams and Trajmar [6] and the previously available close-coupling calculations of Mitroy and McCarthy [7] for all three excitations measured. In order to further test the RDW method and to compare with the new experimental DCS results of Predojević *et al.* [1], we have extended our previous RDW calculations to the excitation of the $3s4s\ ^1S_0$ and $3s4p\ ^1P_1$ states using extensive multiconfiguration wave functions.

Details of the RDW method as applied to Mg are given in Ref. [4] with additional information of the wave functions used in Refs. [2,3]. Here we will concentrate on the details of the wave functions used in the calculations. The initial ground state of magnesium has the configuration $1s^22s^22\bar{p}^22p^43s^2$ in the relativistic j-j-coupling notation where $\bar{p}$ represent a p electron with total (orbital plus spin) angular momentum $j=\frac{1}{2}$ while p represents a p electron with $j=\frac{3}{2}$. In the final states one of the valence $3s$ electrons is excited to a $4s$ or $4p$ level. Even in the simplest representation, the $4p$ level is a linear combination of the $3s4\bar{p}$ and $3s4p$ configurations in j-j coupling. However, in order to obtain wave functions with accurate energies and oscillator strengths, one must carry out a more elaborate configuration-interaction calculation including a number of configurations with the same parity and total angular momentum J. In this work we have used the GRASP92 program [8] to carry our Dirac-Fock calculations. The ground state and $3s4s\ ^1S_0$ excited state both have $J=0$ and even parity. These wave functions were constructed out of the configurations $3s^2$, $3s4s$, $3s5s$, $3\bar{p}^2$, $3p^2$, $3\bar{p}4\bar{p}$, $3p4p$, $3\bar{p}5\bar{p}$, $3p5p$, $3\bar{d}^2$, $3d^2$, $4s^2$, $4\bar{p}^2$, and $4p^2$ which gave an energy of 5.390 eV, very close to the experimental value of 5.394 eV [9]. The $3s4p\ ^1P_1$ state with $J=1$ and odd parity contained the configurations $3s3\bar{p}$, $3s3p$, $3s4\bar{p}$, $3s4p$, $3s5\bar{p}$, $3s5p$, $3\bar{p}3\bar{d}$, $3p3\bar{d}$, $3p3d$, $3\bar{p}4s$, $3p4s$, $3\bar{p}4\bar{d}$, $3p4\bar{d}$, $3p4d$, $3\bar{p}5s$, $3p5s$, $3\bar{d}4\bar{p}$, $3\bar{d}4p$, $3d4p$, $4s4\bar{p}$, $4s4p$, $4s5\bar{p}$, $4s5p$, $4\bar{p}4\bar{d}$, $4\bar{p}5s$, $4p4\bar{d}$, $4p4d$, and $4p5s$ yielding an energy of 6.008 eV compared with the experimental value of 6.118 eV [9]. The calculated value of the oscillator strength for transitions from this state to the ground state was 0.110 in the Babushkin (length) gauge which is well within the error bars of the measured value of 0.113 [9]. It is this quantity that determines the magnitude of the DCS at small scattering angles. The value of the oscillator strength obtained in the Coulomb (velocity) gauge was 0.111 in almost perfect agreement with the Babushkin value

Predojević *et al.* [1] made measurements at 10, 20, 40, and 60 eV incident electron energies while Williams and Trajmar [6] measured only at 20 and 40 eV. Mitroy and McCarthy [7] reported results at 10, 20, 40, and 100 eV. We consider 10 eV too low an energy for our RDW approximation and thus show results at 20, 40, 60, and 100 eV compared to the previous work. In Fig. 1 we present results for the DCS for excitation of the $3s4s\ ^1S_0$ states. Overall our results agree quite well with the calculations of Mitroy and McCarthy [7] except in the region of the first minimum. Also our cross sections show a peak at very small scattering angles which is more characteristic of an optically forbidden transition than the strong forward peak in Ref. [7]. The agreement with the measurements of Predojević *et al.* [1] and Williams and Trajmar [6] are reasonable over much of the angular range but tend to get worse as the energy increases. Figure 2 shows DCS results for the excitation of the $3s4p\ ^1P_1$ state. Out calculations agree quite well with the CC results of Mitroy and McCarthy [7] although there are some differences for scattering angles greater than 70° at 20 eV. We observe a good agreement between the RDW results and the measurements of Predojević *et al.* [1] at small scattering angles. At 20 eV both the experimental and theoretical results are in reasonable agreement over the whole angular range but at 40 and 60 eV, both sets of measurements lie somewhat below the calculations for scattering angles greater than 10° though the shapes of the cross sections are similar.

We also present our results for the integrated cross sections (ICS) in Tables I and II and compare them with the experimental results [1,6] as well as the close-coupling cal-

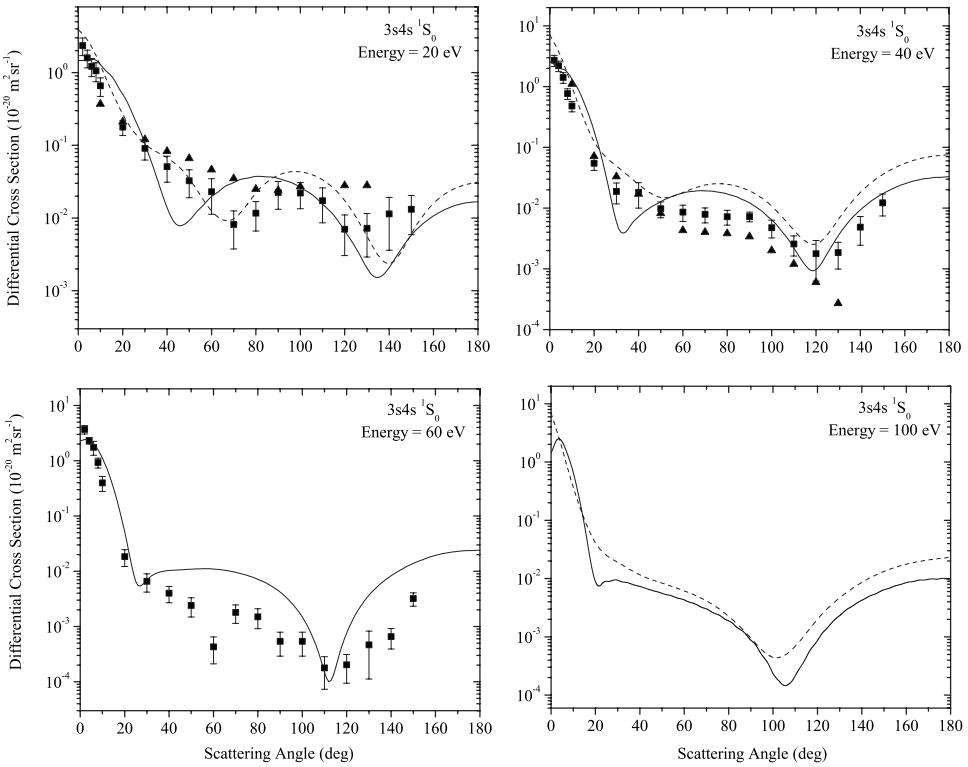

FIG. 1. Differential cross sections for the excitation of the $3s4s$ $^1S_0$ state of Mg by electron impact at 20, 40, 60, and 100 eV. Solid line: present RDW results; dashed line: CC results of Ref. [5]; squares with error bars: measurements of Ref. [1]; triangles: measurements of Ref. [4].

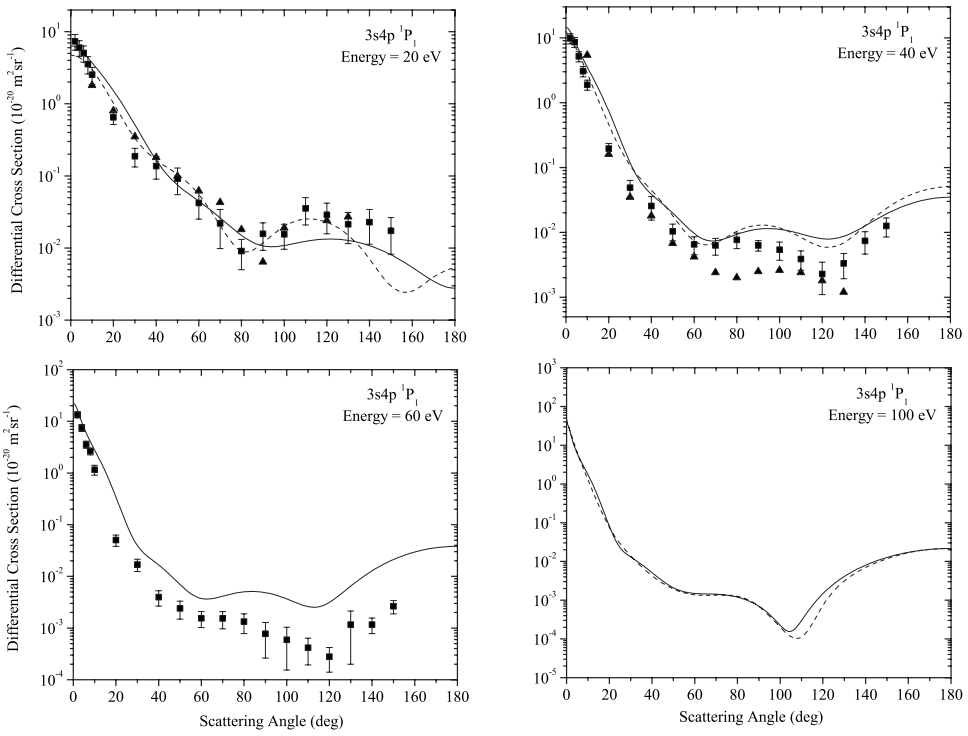

FIG. 2. As for Fig. 1 but for the excitation of the $3s4p$ $^1P_1$ state of Mg.

TABLE I. Integrated cross sections (in units of 10^{-20} m^2) for the excitation of the $3s4s\ ^1S$ state of Mg. RDW indicates the present results. The table also includes results from the two experimental measurements [1,6] as well as the close-coupling calculations of Ref. [7].

Energy (eV)	RDW	Experiment [1]	Experiment [6]	CC [7]
20	0.665	0.495 ± 0.188	0.6	0.76
40	0.488	0.277 ± 0.077	0.3	0.59
60	0.359	0.198 ± 0.056		
100	0.228			0.23

culations of Ref. [7]. Note that the experimental DCS have to be extrapolated to both forward and backward scattering angles before integrating them to obtain the ICS. Since the ICS is dominated by contributions from the DCS at small scattering angles our results are somewhat higher than the experimental ones and tend to approach the close-coupling results as the incident electron energy increases as can be inferred from our DCS results.

We have carried out fully relativistic calculations for the electron excitation $3s4s\ ^1S_0$ and $3s4p\ ^1P_1$ states of magnesium at intermediate scattering energies and compared them with previous experimental [1,6] and theoretical work [7]. Overall, we confirm the earlier calculations [7] and while our results are not dissimilar to the experimental data [1], the discrepancies at larger scattering angles tend to widen as the scattering energy increases.

TABLE II. As for Table I for the excitation of the $3s4p\ ^1P$ state of Mg.

Energy (eV)	RDW	Experiment [1]	Experiment [6]	CC [7]
20	2.01	1.39 ± 0.45	1.3	1.63999
40	1.42	0.805 ± 0.189	1.2	1.14581
60	1.07	0.541 ± 0.121		
100	0.725			0.66094

A.D.S. would like to thank NSERC Canada for a research grant in partial support of this work. L.S. is thankful to the Ministry of Human Resource Development (MHRD), India, for financial assistance.

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