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Electron scattering by magnesium: excitation of the 3s3p $^1P_1$ state

D M Filipović[1,2], B Predojević[1,3], V Pejčev[1,4], D Šević[1], B P Marinković[1], Rajesh Srivastava[5] and A D Stauffer[6]

[1] Institute of Physics, PO Box 68, 11080, Belgrade, Serbia and Montenegro
[2] Faculty of Physics, University of Belgrade, PO Box 368, 11001, Belgrade, Serbia and Montenegro
[3] Faculty of Natural Sciences, University of Banja Luka, Republic of Srpska, Bosnia and Herzegovina
[4] Faculty of Natural Sciences, University of Kragujevac, 34000 Kragujevac, Serbia and Montenegro
[5] Department of Physics, Indian Institute of Technology, Roorkee-247667, India
[6] Department of Physics and Astronomy, York University, Toronto M3J 1P3, Canada

E-mail: bratislav.marinkovic@phy.bg.ac.yu

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Abstract

Differential cross sections (DCS) for electron-impact excitation of the 3s3p $^1P_1$ state in magnesium at incident electron energies $E_0 = 10$, 15, 20, 40, 60, 80 and 100 eV have been measured and corresponding calculations carried out. Scattered-electron intensities were measured over a wide range of scattering angles (10°–150°) and normalized to the DCSs at 10° experimentally obtained by Filipović *et al* (2006 *Int. J. Mass Spectrom.* **251** 66). Corresponding calculations have been conducted in the relativistic distorted-wave approximation. Integrated (integral, momentum transfer and viscosity) cross sections are determined by numerical integration of our DCSs. The results are analysed and compared with previous experimental data and theoretical calculations.

1. Introduction

Following our investigation of electron scattering by Yb, Hg, Cd, Zn and Ca (Predojević *et al* 2005a, 2005b and references therein), we have extended our studies of two valence electron atoms to Mg. Magnesium is identified as the lightest quasi-two-electron atom that may serve as a rigorous test of new methods in scattering theory. Beryllium is not considered because it is very toxic. Also, in order to understand radiation damage of biomolecules

caused by the secondary low energy electrons (Sanche 2002), a knowledge of binary electron–atom collision processes is required. Magnesium is the central atom in chlorophyll, MgATP molecules provide energy for almost all metabolic processes, and it is required at a number of steps during the synthesis of DNA, RNA and proteins.

In this paper, we continue our study of the 3s3p $^1P_1$ state of magnesium excited from the ground by electron impact. Recently (Filipović *et al* 2006), we have reported absolute experimental differential cross sections (DCS) at incident electron energies $10 \leqslant E_0$ (eV) $\leqslant 100$ and small scattering angles $2^\circ \leqslant \theta \leqslant 14^\circ$, together with theoretical results obtained using the relativistic distorted-wave (RDW) approximation. Very good agreement was obtained at small scattering angles between these experimental data and the calculated DCSs using elaborate multi-configuration wavefunctions for the atomic states. Thus, we established the experimental DCSs at 10° as a base for the normalization of our present relative measurements of the DCSs which are extended over a wide range of scattering angles up to 150°. In this way, we obtained absolute DCS values which were extrapolated to 0° and 180° and numerically integrated to yield the integral (Q_I), momentum transfer (Q_M) and viscosity (Q_V) cross sections as defined in Marinković *et al* (1991). Fano plots (Fano 1954) were also utilized for the analysis of the integral cross sections.

There are only a few papers containing experimental data of electron scattering on magnesium atoms. Williams and Trajmar (1978) measured DCSs for the excitation of the 3s3p $^1P_1$ state, including elastic and several other inelastic ones at impact energies of 10, 20 and 40 eV and scattering angles from 10° to 130°. For the normalization of the relative DCSs they chose the excitation function of Leep and Gallagher (1976). The same normalization procedure has been applied by Brunger *et al* (1988) to measured DCSs for the 3s3p $^1P_1$ state at energies of 10 eV and 20 eV (from 3° to 130°) and at 40 eV (from 5° to 130°). Recently, Brown *et al* (2005) reported their scattered-electron–polarized-photon results for the excitation of the resonance state in magnesium by 20 eV incident electrons, adding DCSs at scattering angles from 10° to 140° to the previously reported studies at 40 eV (Brown *et al* 2003). They have also included convergent close-coupling (CCC) and *R*-matrix with pseudo-states calculations and normalized the relative experimental DCSs at impact energies mentioned above to the CCC results so as to give a best visual fit.

Calculations of the DCS and Q_I cross sections for magnesium have been carried out by Fabrikant (1980) for the $3s^2\,{}^1S_0 \rightarrow 3s3p\,{}^1P_1$ transition at $E_0 = 10$ and 20 eV, using the two-state close-coupling (CC2) approximation. Mitroy and McCarthy (1989) computed DCSs for the excitation of the four lowest singlet states (3s3p $^1P_1$, 3s4s $^1S_0$, 3s4d $^1D_2$ and 3s4p $^1P_1$) and for elastic scattering at $E_0 = 10$, 20, 40 and 100 eV, using the five-state close-coupling (CC5) approximation. They also calculated the integral cross sections for the excitation of the resonance transition including cascade contributions at all energies studied. McCarthy *et al* (1989) calculated DCSs and Q_I cross sections for inelastic (the excitation of the 3s3p $^1P_1$ and $^3P_1$ states) and elastic scattering at $E_0 = 10$, 20 and 40 eV using six-state close-coupling (CC6 and optical CCO6) methods. Meneses *et al* (1990) used first-order many-body theory (FOMBT) to calculate DCSs for the excitation of the 3s3p ($^1P_1$ and $^3P_1$) states at $E_0 =$ 20, 30, 40, 50 and 100 eV. Clark *et al* (1991) used both FOMBT and distorted-wave (DW) approximations to study the influence of target-state wavefunctions on DCS (at 10 and 40 eV) and Q_I (from 10 to 100 eV) results for the 3s3p $^1P_1$ state. Kaur *et al* (1997) applied the relativistic distorted-wave (RDW) approximation to calculate DCSs for the 3s3p ($^1P_1$ and $^3P_{0,1,2}$), 3s3d ($^1D_2$ and $^3D_{1,2,3}$) and 3s4p ($^1P_1$ and $^3P_{0,1,2}$) states in magnesium at $E_0 = 10$, 20 and 40 eV. Fursa and Bray (2001) calculated DCSs for electron-impact excitation of the 3s3p $^1P_1$ state at $E_0 = 10$, 20 and 40 eV using the 27-state (CC27) CCC approach. Gedeon *et al* (1998) employed the *R*-matrix method in the calculation of integral cross sections for

the $3s^2\,{}^1S \rightarrow 3s3p\,{}^1P$ and $3s^2\,{}^1S \rightarrow 3s3p\,{}^3P$ transitions from threshold to 30 eV impact energies.

In section 2, the apparatus is described and the experimental procedure is given. In section 3, the RDW method as applied to the DCS calculation is outlined. In section 4, present absolute DCS values and integrated (Q_I, Q_M and Q_V) cross sections are tabulated, and presented graphically together with other measurements and calculations for comparison. Finally, in section 5, our results are discussed and conclusions given.

2. Apparatus and experimental procedure

A conventional cross-beam electron spectrometer designed for metal atom targets, housed in a magnetically shielded differentially pumped vacuum chamber, was used to obtain the magnesium DCS data. The spectrometer has been used recently to record energy-loss spectra and measure DCSs in Yb (Predojević *et al* 2005a, 2005b), Ca (Milisavljević *et al* 2005) and Zn (Fursa *et al* 2005). Only a brief description of the apparatus is given here with more details relating to magnesium as a target. The spectrometer is utilized for recording the electron energy-loss spectra from 0 eV to slightly above the ionization potential (IP) at 7.646 eV and direct angular distribution measurements of the inelastically scattered electrons over a wide range of scattering angles up to 150°. A channel electron multiplier is utilized for single-electron counting. An overall system energy resolution (as FWHM) of 120 meV was maintained for these measurements. In a separate experiment, the excitation function mode of operation with a resolution of about 50 meV was applied to calibrate the energy scale against the $3s3p\,{}^1P_1$ excitation threshold at 4.346 eV. The influence of the contact potential difference between the thoriated tungsten filament (work function of Th is $W = 3.4$ eV) and the magnesium-plated ($W = 3.66$ eV) collision chamber on the energy scale is low. The uncertainty in the energy was estimated to be less than 0.1 eV. The real zero scattering angle was determined on the basis of the symmetry of the scattered-electron intensity with respect to the mechanical zero within a 0.2° uncertainty. The angular resolution of the spectrometer is estimated to be 1.5° (2° at 10 eV).

The construction of the resistively heated oven for producing and controlling the magnesium vapour beam was the same as previously reported (Filipović *et al* 2006). The measurements were performed at a temperature of 780 K for magnesium of 99.9% purity. The number density of the atom beam effusing through the cylindrical channel (aspect ratio $\gamma = 0.075$) from the oven was not measured, but was estimated to be typically 10^{13}–10^{14} cm^{-3}. Water cooling of the oven shield together with thermal insulation by ceramics protected the channel electron multiplier from a rise in temperature.

Relative DCSs for the $3s3p\,{}^1P_1$ state were obtained by direct angular distribution measurements. Briefly, for a given E_0, the position of the analyser was changed from 10° to 150° and the scattered-electron intensity was directly measured. The scattering intensity was corrected using the effective path-length correction factors according to the approach of Brinkman and Trajmar (1981). In this work, we used our experimental absolute DCS values at 10° (Filipović *et al* 2006) to put these relative DCSs on an absolute scale.

Contributions to the total error of the absolute DCSs come from: (a) uncertainties in our experimental values and (b) uncertainty in the normalization procedure. The errors in our experimental values arise from statistical errors, and uncertainty of the effective path-length correction factor (<0.06, i.e. 6%), energy (0.01) and angle (<0.10) as mentioned above. The uncertainty in the normalization procedure (0.10) is assumed to be the same as derived in the procedure for the determination of DCSs at 10° used here as the normalization points.

3. Calculation method

The theoretical basis of our calculations for magnesium was given by Kaur *et al* (1997) while the details of the wavefunctions used were discussed in our previous publication (Filipović *et al* 2006). We briefly review here the main points of the calculations.

The RDW method is based on the consistent use of the Dirac equations for both the target wavefunctions and the scattered waves. These are particularly well suited for scattering from heavy atoms but can be equally well applied to light atoms such as magnesium. While we would expect calculations based on the non-relativistic Schroedinger equation to yield comparable results in this case, there is an advantage to using a consistent theoretical method which is applicable to atomic systems whatever their nuclear charge. In particular, this allows for meaningful comparisons among the calculations for two-electron systems whose nuclear charges can vary substantially. The target is represented by Dirac–Fock wavefunctions calculated using the GRASP92 program of Parpia *et al* (1996). In the *j–j* coupling notation, the ground $^1S_0$ state configurations of magnesium is $1s^2 2s^2 2\bar{p}^2 2p^4 3s^2$ where $\bar{p}$ and p indicate p-electrons with total angular momenta j of $1/2$ and $3/2$, respectively. The excited $^1P_1$ state is a linear combination of the $3s3\bar{p}$ and 3s3p valence configurations. These are the basis of our simple single-configuration ground-state (SCGS) calculation. We have also used more elaborate wavefunctions where we have added to these basic spectroscopic configurations the valence configurations 3s4s, $3\bar{p}^2$, $3\bar{p}4\bar{p}$, $3p^2$, 3p4p, $3\bar{d}^2$ and $3d^2$ in the ground state and the valence configurations $3s4\bar{p}$, 3s4p, $3\bar{p}3\bar{d}$, $3\bar{p}4s$, $3p3\bar{d}$, 3p3d and 3p4s in the excited state. We designate these as multi-configuration ground-state (MCGS) results. These latter wavefunctions give excellent energies and an accurate oscillator strength for the transition.

The distorted waves in the incident and scattered channels are calculated from the Dirac equations using the static potential of the excited state as a distortion potential. From these we can evaluate the scattering amplitudes and hence the DCSs as detailed in Kaur *et al* (1997) and Filipović *et al* (2006).

4. Results

An energy-loss spectrum of magnesium at 60 eV incident electron energy and scattering angle of 10° is shown in figure 1, together with the spectrum at 10 eV and 10° in the inset. The spectra contain well-resolved features that correspond to the elastic scattering, 3s3p $^1P_1$ (resonant state at $\Delta E = 4.346$ eV) and also the 3s4s $^1S_0$, 3s3d $^1D_2$ and 3s4p $^1P_1$ states. The 3s3p ^3P peak at $\Delta E = 2.71$ eV is weaker than a very low background signal in this higher energy–low angle 'optical-like' spectrum, but it is clearly recognized in the inset.

We have measured relative differential cross sections for electron-impact excitation of the 3s3p $^1P_1$ state in magnesium at incident electron energies of 10, 15, 20, 40, 60, 80 and 100 eV. The present absolute DCSs were obtained using absolute DCS values at $\theta = 10°$ from Filipović *et al* (2006) as explained in section 2. The absolute DCS values (with total errors in the parenthesis) are given in table 1 and presented graphically (with corresponding statistical errors indicated) in figures 2 and 3 together with the present RDW calculations. Also included in the same figures are DCSs measured by Williams and Trajmar (1978) and Brunger *et al* (1988) and calculated using the CC5 (Mitroy and McCarthy 1989) and CCC (Fursa and Bray 2001, Fursa 2005) approximations. For the sake of clarity, several of the theoretical results mentioned in the introduction are not shown in the figures.

Our experimental integrated cross sections are obtained by the extrapolation of the absolute DCSs to 0° using our previously reported results at small angles and to 180° using the shape of our calculated DCSs to fit the experimental data for scattering angles $\theta > 140°$ followed by

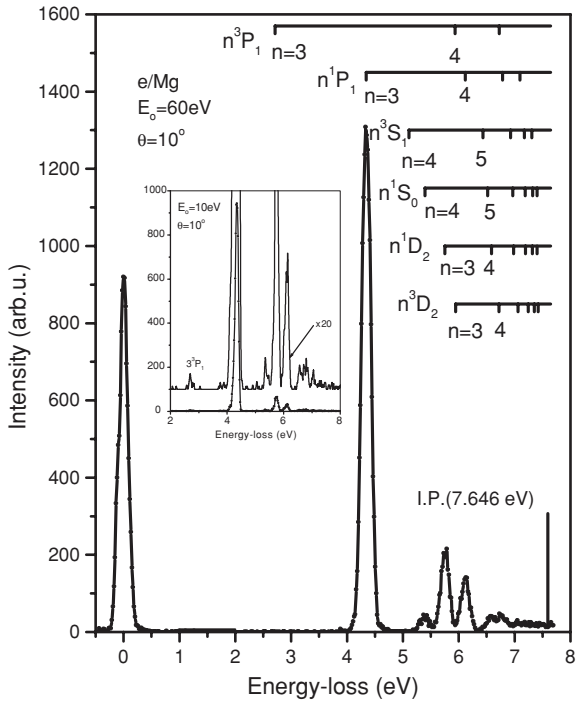

Figure 1. Electron energy-loss spectrum of Mg at $E_0 = 60$ eV impact energy and scattering angle $\theta = 10^\circ$ which represents an 'optical-like' spectrum. The inset shows the details of the spectrum at lower energy ($E_0 = 10$ eV) in the region of the $3s3p^3P$ and higher excited states.

numerical integration. The total errors arise from separate DCS errors, and the extrapolation of DCSs and numerical integration (0.1). The values of Q_I, Q_M and Q_V are given at the bottom in table 1, with total errors in the parenthesis.

5. Discussion and conclusion

Very good agreement between our experimental and calculated DCS data for the resonant $3s3p\ ^1P_1$ state of magnesium at $10 \leqslant E_0$ (eV) $\leqslant 100$ and small scattering angles $2^\circ \leqslant \theta \leqslant 14^\circ$ reported recently indicates the validity of the RDW models in the case of the lightest quasi-two-electron atom. At 40 eV impact energy, the measured DCS clearly exhibits two minima around 60° and 120° which agree very well with the location of the minima predicted by all the theories. At 20 and 10 eV, there is disagreement among the theories as to whether there are one or two minima in the DCS. At 20 eV, our measurements support the existence to two minima but at 10 eV only the minimum at 100° is clearly seen. To the best of our knowledge, DCSs for the $3s3p\ ^1P_1$ state of magnesium at the energies of 15, 60 and 80 eV are obtained for the first time in this work. Our RDW MCGS calculations produce data in very good agreement with the present experimental DCSs at small angles and are superior to our SCGS calculations at almost all scattering angles and energies. At $E_0 = 100$ eV, the theoretical minimum is narrow enough for the discrepancy to be mostly due to the experimental angular and energy resolution.

Table 1. Differential cross sections (in units of 10^{-20} m^2 sr^{-1}) for electron-impact excitation of the 3s3p ^{1}P$_1$ state of magnesium atom. The last three rows present integral (Q_I), momentum transfer (Q_M) and viscosity (Q_V) cross sections in units of 10^{-20} m^2. The absolute errors are indicated in parentheses.

Scattering angle (°)	DCS ($\times 10^{-20}$ m^2 sr^{-1})						
	10 eV	15 eV	20 eV	40 eV	60 eV	80 eV	100 eV
5	41.9(6.9)	95.6(14.8)	115(18)	141(22)	103(16)	95.2(14.7)	85.3(13.1)
10	28.8(4.4)	39.8(6.1)	41.8(6.5)	27.3(4.2)	12.6(1.9)	11.0(1.7)	6.79(1.06)
20	8.45(1.30)	6.71(1.03)	5.66(0.87)	2.06(0.32)	0.415(0.066)	0.309(0.048)	0.171(0.027)
30	3.09(0.48)	1.32(0.21)	1.25(0.19)	0.442(0.069)	0.0941(0.0161)	0.0724(0.0114)	0.0361(0.0060)
40	1.43(0.22)	0.465(0.074)	0.586(0.091)	0.156(0.025)	0.0314(0.0063)	0.0224(0.0037)	0.0122(0.0020)
50	0.699(0.109)	0.244(0.039)	0.273(0.043)	0.0725(0.0123)	0.0190(0.0043)	0.0145(0.0024)	0.006 54(0.001 00)
60	0.381(0.059)	0.108(0.019)	0.126(0.021)	0.0632(0.0108)	0.0166(0.0039)	0.0120(0.0020)	0.006 66(0.001 00)
70	0.151(0.025)	0.0391(0.0069)	0.0914(0.0152)	0.0714(0.0121)	0.0102(0.0028)	0.0101(0.0017)	0.003 84(0.000 93)
80	0.102(0.017)	0.0349(0.0063)	0.0872(0.0146)	0.0672(0.0115)	0.0111(0.0024)	0.006 19(0.001 10)	0.001 85(0.000 54)
90	0.0821(0.0138)	0.0346(0.0063)	0.114(0.019)	0.0471(0.0034)	0.007 34(0.001 79)	0.002 89(0.000 57)	$7.92 \times 10^{-4}(2.88 \times 10^{-4})$
100	0.0645(0.0111)	0.0360(0.0065)	0.107(0.018)	0.0335(0.0062)	0.003 46(0.001 09)	$8.20 \times 10^{-4}(2.00 \times 10^{-4})$	$6.39 \times 10^{-4}(2.42 \times 10^{-4})$
110	0.0769(0.0130)	0.0426(0.0075)	0.0965(0.0160)	0.0201(0.0041)	$9.52 \times 10^{-4}(5.22 \times 10^{-4})$	$9.73 \times 10^{-4}(2.30 \times 10^{-4})$	0.001 19(0.000 35)
120	0.0735(0.0125)	0.0332(0.0060)	0.0753(0.0127)	0.0080(0.0021)	0.001 80(0.000 74)	0.003 56(0.000 68)	0.003 56(0.000 78)
130	0.0637(0.0110)	0.0281(0.0052)	0.0576(0.0100)	0.0204(0.0042)	0.009 13(0.002 09)	0.0114(0.0019)	0.006 94(0.001 00)
140	0.0673(0.0116)	0.0217(0.0042)	0.0719(0.0122)	0.0408(0.0074)	0.0149(0.0032)	0.0236(0.0038)	0.0103(0.0020)
150	0.0625(0.0108)	0.0168(0.0035)	0.101(0.017)	0.0642(0.0110)	0.0306(0.0062)	0.0463(0.0075)	0.0212(0.0040)
Q_I	14.0(2.2)	14.9(2.7)	16.6(2.6)	14.2(2.6)	10.6(1.7)	9.90(1.55)	9.47(1.48)
Q_M	4.91(0.79)	3.13(0.59)	3.52(0.57)	1.49(0.27)	0.646(0.098)	0.561(0.090)	0.339(0.056)
Q_V	7.41(1.17)	5.24(0.97)	5.00(0.79)	2.21(0.41)	1.01(0.16)	0.710(0.112)	0.514(0.083)

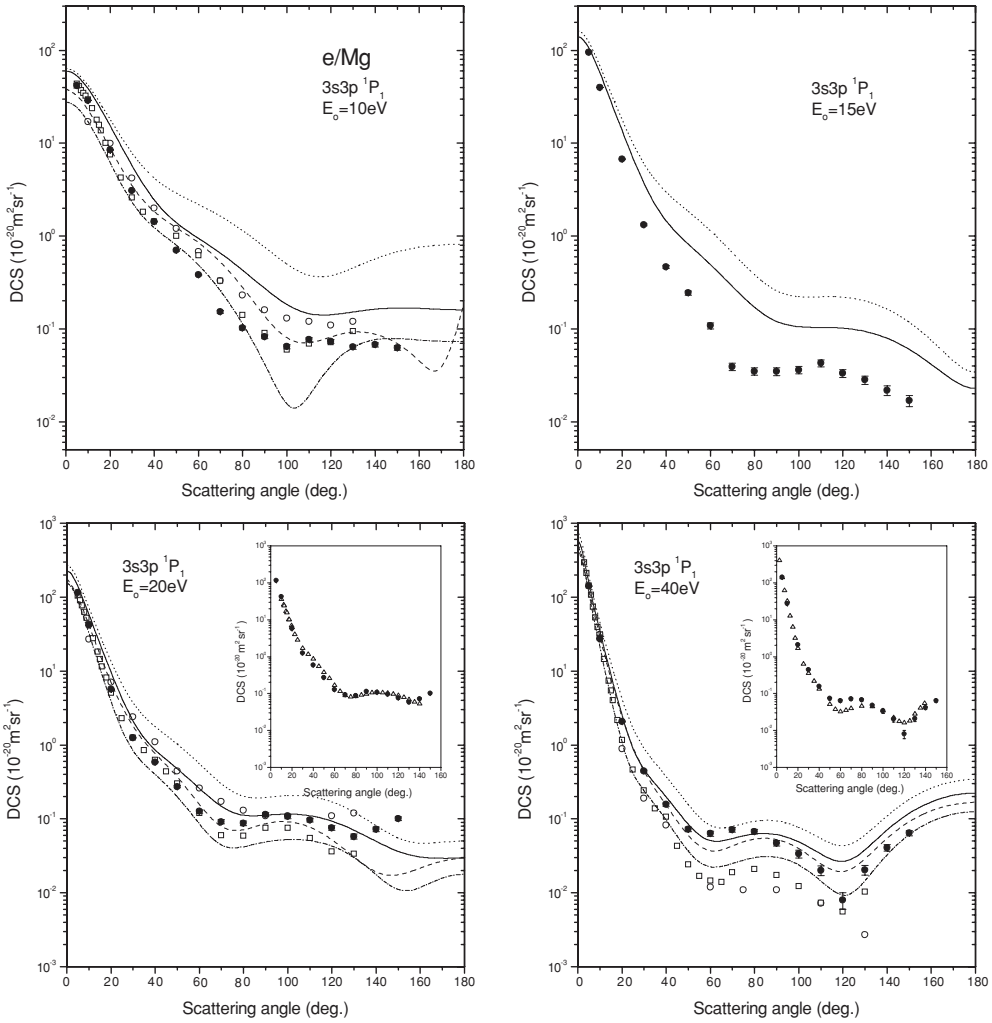

Figure 2. Differential cross sections (DCS) for electron-impact excitation of the 3s3p $^1P_1$ state of Mg atom at 10, 15, 20 and 40 eV impact energies. Present: (•) experiment (total error bars are indicated); (—) RDW MCGS calculation; (· · ·) RDW SCGS calculation. Other results: (○) Williams and Trajmar (1978); (□) Brunger *et al* (1988); (– – –) CC5 (Mitroy and McCarthy 1989); (– · –) CCC (Fursa and Bray 2001, Fursa 2005). Insets show the results (△) at 40 eV and 20 eV of Brown *et al* (2003, 2005), respectively, both normalized to the present experimental DCS at 100°.

Our experimental DCSs are in better agreement both in shape and magnitude with those of Brunger *et al* (1988) than with those of Williams and Trajmar (1978). We found that our DCSs decrease at larger angles at 10 and 15 eV, but the second minimum appears at 130° for 20 eV, 120° for 40 eV, 110° for 60 eV, between 100° and 110° for 80 eV and 100° for 100 eV impact energy. The agreement with the recent experimental DCS for 20 eV by Brown *et al* (2005) normalized to our DCS at 100° is excellent (left inset in figure 2) except at the highest angle measured by these authors. The right inset in the same figure shows the DCS at 40 eV by Brown *et al* (2003) normalized at 100° to our corresponding DCS obtained as the arithmetic mean of six independent measurements. The second minimum is deeper in our measurements, but the first minimum is not deep enough to be in accord with most of the other results.

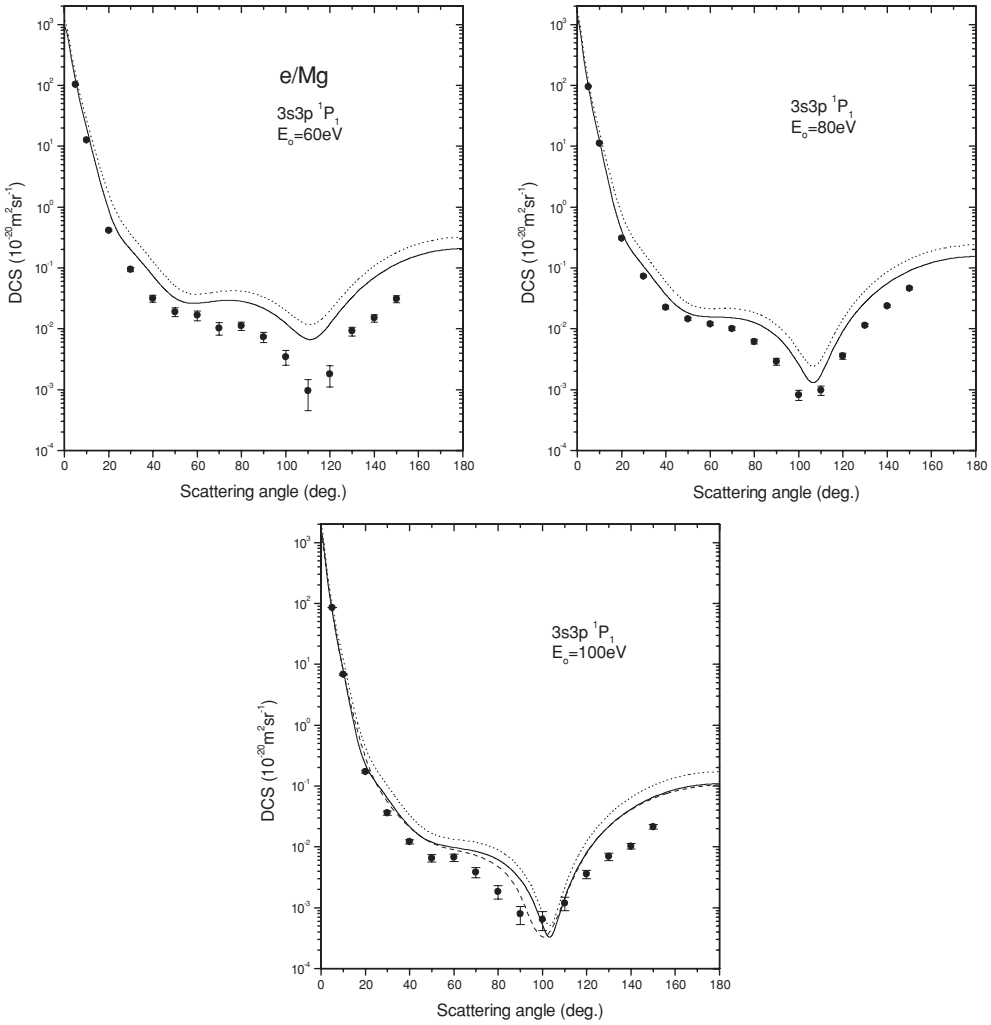

Figure 3. Same as figure 2, but at 60, 80 and 100 eV incident electron energies.

As one can see in figure 4, our experiment is in agreement with previous experiment (Leep and Gallagher 1976; while the absolute measurement by Aleksakhin *et al* (1973) is not considered because of the low cross-section values) and the calculations of Mitroy and McCarthy (1989) and Clark *et al* (1991), and matches the present RDW MCGS calculations at higher energies. The SCGS results are clearly too large as expected from the poor value obtained for the optical oscillator strength. Going towards lower impact energies, the present RDW MCGS calculation overestimates the present experiment in contrast to the CCC results by Fursa and Bray (2001) that underestimates our measurements by a similarly amount.

To compare Mg with other atoms studied in our laboratory, that also have two valence electrons, we considered a general rule that effective cross section for electron/atom impact is lower if the ionization potential is higher, as it is noted in paper dealing with Zn and Cd (Predojević *et al* 2003). We found that this rule is valid in the case of electron-impact excitation of the resonant n^1P states of Mg and Ca (Milisavljević *et al* 2004) for $n = 3$

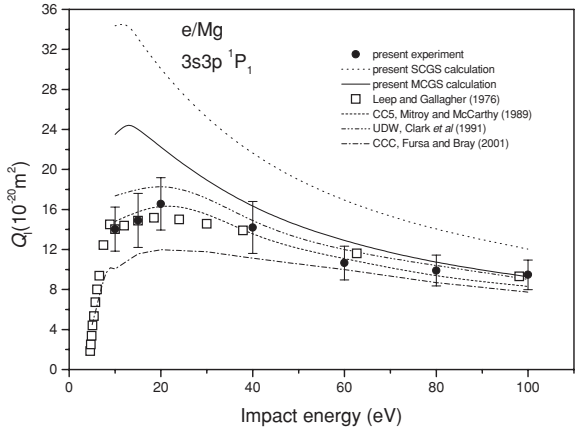

Figure 4. Integral cross sections for electron-impact excitation of the 3s3p $^1P_1$ state of magnesium atom.

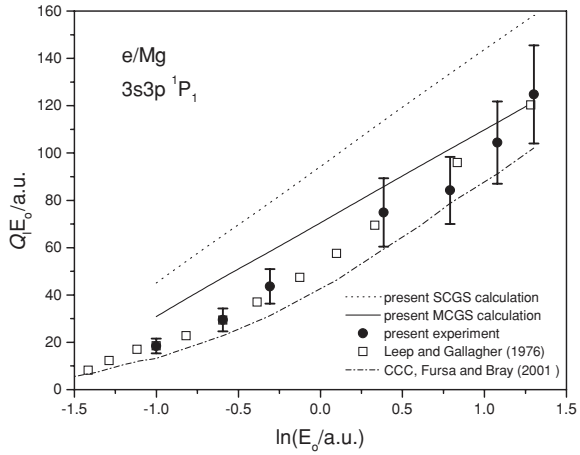

Figure 5. Fano plot for the 3s3p $^1P_1$ state of magnesium. Product of the integral cross section (Q_I) and incident electron energy (E_0) versus logarithm of E_0, both are given as traditionally in atomic units.

and 4, respectively. Additional analysis of the integral cross sections using a Fano plot (figure 5) has provided a check of this conclusion. The Fano plot obtained from the excitation functions of Leep and Gallagher (1976) is consistent with our experiment, as well as with our MCGS results at higher energies.

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