J. Phys. B: At. Mol. Opt. Phys. 27 (1994) 3573–3580. Printed in the UK

Electron impact excitation of the 3^3P state in magnesium

R K Houghton, M J Brunger, G Shen† and P J O Teubner

Institute for Atomic Studies, School of Physical Sciences, The Flinders University of South Australia, Bedford Park, South Australia, 5042, Australia

Received 16 May 1994, in final form 7 June 1994

Abstract. A modulated crossed beam technique has been used to measure the differential cross sections for the excitation of the 3^3P state in magnesium by electrons at impact energies of 10 and 20 eV. The cross sections are measured over a range of scattering angles from 10 to 130°. Our results agree with the previous experimental cross sections of Williams and Trajmar within the combined uncertainties, however the present data reduce the uncertainty by almost an order of magnitude thereby allowing a meaningful comparison to be made with the predictions of the various theories. At this time no theory accurately predicts the behaviour of the cross sections over the whole angular range.

1. Introduction

The electron impact excitation of magnesium from the ground state to the 3^3P state may occur either by the spin–orbit interaction, the exchange interaction or by a combination of these two physical processes. As magnesium is a relatively light atom ($Z = 12$) we would *a priori* expect deviation from pure *LS* coupling to be small. Indeed, Kuhn (1969) has explicitly demonstrated this to be the case. Consequently we would expect the population of the 3^3P state to be dominated by exchange processes. Hence a measurement of the differential cross section for the electron impact excitation of the 3^3P state in magnesium not only provides an important general test for the various theories attempting to describe the scattering process but, in particular, it probes these models for their treatment of electron exchange.

The previous measurements of Williams and Trajmar (1978) were subject to large (±50%) uncertainties in the cross sections. Thus it has not been possible to test the predictions of the theory. McCarthy *et al* (1989) have reported a series of calculations on the excitation of the 3^3P state based on a six state close coupling approximation. These calculations also included a continuum optical model (CCOM). More recently Zhou (1994) extended this work to a ten-state calculation which incorporated higher order singlet states (5^1S, 5^1P) and higher order triplet states (4^3S, 4^3P). Meneses *et al* (1990) have applied a first-order many-body theory (FOMBT) to the problem. For impact energies of both 10 eV and 20 eV there is a difference of about a factor of two at forward angles in the predicted cross sections of the many body and close coupling theories. This difference cannot be resolved by the previous measurements. The predictions of each of these theories also disagree with those from a perturbation theory calculation of Avdonina and Amuy'sa (1983). Thus it is appropriate to provide a set of measured differential cross sections with uncertainties which permit meaningful comparisons with the theories. We have, therefore,

† Present address: Defence Scientific and Technology Organisation, Salisbury, SA 5108, Australia.

0953-4075/94/153573+08$19.50

measured cross sections for the excitation of the 3^3P state in magnesium over the angular range from 10° to 130° at incident electron energies of 10 eV and 20 eV.

The experimental procedure is described in section 2 whilst our results are presented and discussed in section 3.

2. Experimental techniques

The modulated cross beam apparatus used in this experiment has been described in detail previously (see Brunger *et al* 1988). Briefly, a magnesium beam intersects an electron beam at right angles in the scattering chamber to define an interaction region. The magnesium beam was produced by a multichannel array in a Joule heated oven which was operated at a temperature of about 536 °C. The magnesium beam was further collimated by two apertures before reaching the interaction region where the beam density was approximately 1.72×10^{15} m^{-3}. A cylindrical mirror electron spectrometer viewed the interaction region.

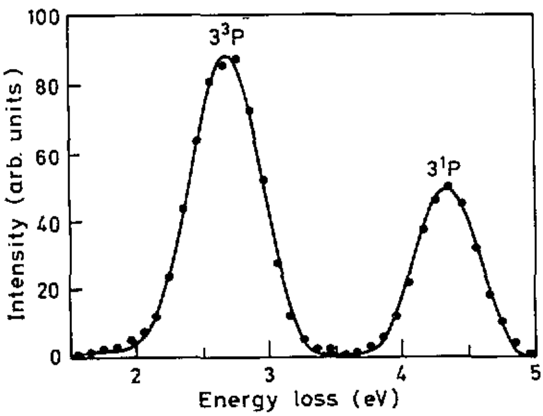

Figure 1. Typical energy loss spectra. $E_0 = 10$ eV and $\theta_e = 90°$.

The electron beam was produced by an electron gun which was modified from that previously used (Teubner *et al* 1986) by replacing the tungsten cathode with an oxide cathode. This modification improved the energy resolution of the electron beam to ~ 0.4 eV (FWHM). Stable beam currents of about 1 μA were obtained. The combined energy resolution of the electron beam and spectrometer was 0.8 eV which adequately resolved the 3^3P state from both the ground and the 3^1P states. An energy loss spectrum, reproduced in figure 1, clearly shows that the 3^3P peak at 2.7 eV energy loss is resolved from any other adjacent peak. The energy loss spectra of electrons scattered from magnesium which were taken at each scattering angle showed that the 3^3P state was resolved from the 3^1P state at all angles $\geqslant 10°$.

The energy of electrons scattered through some angle θ were analysed by a cylindrical mirror electron spectrometer and were detected by a channel electron multiplier. The electric field in the spectrometer was set so that electrons which had lost 2.7 eV were detected in the channeltron. Pulses from the channeltron were amplified and counted in either of two gated scalers. The modulation of the magnesium beam by a rotating toothed wheel provided a reference signal to gate the scalers. One scaler was enabled when the neutral beam was in the interaction region, that is, it counted the scattered signal from both the beam and the background, N_a. The other scaler, enabled when the beam was off, counted the scattered signal only from the background, N_b.

Both scalers counted for a preset time and the difference

$$N = N_a - N_b \tag{1}$$

was proportional to the number of electrons which had excited the 3^3P state and scattered from the beam through an angle θ. The relative angular distribution $N(\theta)$, for the excitation of the 3^3P state was obtained by repeating this procedure at each scattering angle.

The relative angular distribution $N(\theta)$ is related to the differential cross section $\sigma(\theta)$ by

$$\sigma_{3^3\mathrm{P}}(\theta) = \frac{N_{3^3\mathrm{P}}(\theta)}{I_0 \rho \eta \tau (\ell \mathrm{d}\Omega)_{\mathrm{eff}}} \tag{2}$$

where I_0 is the incident electron beam current, ρ the target beam density, $(\ell\mathrm{d}\Omega)_{\mathrm{eff}}$ the effective solid angle, η the efficiency of the electron detector and τ the transmission of the spectrometer. In a carefully conducted experiment all of these factors are independent of the scattering angle. Thus by maintaining I_0, ρ and $(\ell\mathrm{d}\Omega)_{\mathrm{eff}}$ constant throughout the experiments equation (2) can be written as

$$\sigma_{3^3\mathrm{P}}(\theta) = C\, N_{3^3\mathrm{P}}(\theta). \tag{3}$$

A similar relationship can be deduced for the 3^1P state, that is

$$\sigma_{3^1\mathrm{P}}(\theta) = C\, N_{3^1\mathrm{P}}(\theta). \tag{4}$$

In this case however the differential cross section is known (Brunger *et al* 1988). Combining equations (3) and (4) yields

$$\sigma_{3^3\mathrm{P}}(\theta_0) = \sigma_{3^1\mathrm{P}}(\theta_0) R_{\theta_0} \tag{5}$$

where R_{θ_0} is the ratio of the scattered signal from the 3^3P state to the 3^1P state at the normalizing angle θ_0.

Equation (5) then fixes the relative angular distribution at the angle θ_0 which consequently determines the differential cross section at all angles θ.

2.1. Discussion of experimental uncertainties

A great deal of care was exercised during these measurements to identify and exclude sources of systematic error.

The temperature of the magnesium beam source was monitored throughout the experiments and was found to vary by less than 1 K over the course of a run. Thus the maximum variation in the atomic beam density was about 2%. The incident electron current was monitored in a Faraday cup. Over the course of a run the incident electron current was found to be constant to within 1%.

The ambient magnetic field in a large volume about the interaction region was reduced to less than 5×10^{-7} T by lining the scattering chamber with μ-metal and using three sets of mutually orthogoral Helmholtz coils. Electrical feedthroughs, cables and insulators were shielded to remove stray electrical fields from the interaction region.

The zero scattering angle was determined by sweeping the spectrometer through the primary electron beam and measuring small angle scattering intensities either side of the electron beam. The zero scattering angle was then defined by the axis of symmetry. This technique was confirmed by measuring the 3^1P angular distribution and comparing with the shape of the 3^1P differential cross section of Brunger *et al* (1988). The scattering angle was then known to within $\pm 0.2°$.

For all scattering angles in the angular range 0° to 130° the spectrometer views a volume at the intersection of the two beams larger than the interaction region. The size of the intereaction region was then independent of the scattering angle. Thus ($\ell d\Omega_{eff}$) the effective solid angle was independent of the scattering angle.

The energy of the incident electron beam was calibrated against the *b* feature in the excitation function for the metastable states in neon at 16.906 eV (Buckman *et al* 1983). This calibration procedure showed that there was a significant difference of 2.4 eV between the cathode potential and the beam energy when the oxide cathode was used as a source of electrons. We estimate that the beam energy is accurate to ± 0.1 eV.

Before the scattered electrons entered the spectrometer, they passed through a three element lens which not only focused the electrons onto a virtual entrance slit but also accelerated them to a constant analysing energy of 20 eV. The final lens ratios for the two groups of scattered electrons at an incident energy of 10 eV was 2.74 and 3.5 respectively whilst at 20 eV the lens ratios were 1.16 and 1.27. A careful study of the lens parameters of Harting and Read (1976) shows that the electron optical settings which were employed were not particularly sensitive to changes in these voltage ratios. This observation was confirmed by measuring the cross section ratios R for a variety of potentials on the mid element lens and the front plate of the spectrometer. It was found that the value of R changed by $< 4\%$ over the range of potentials applied.

Further we note that the triplet and singlet peaks shown in figure 1 have the same full width at half maximum. The resolution of the electron spectrometer depends on the slit width which in this case is determined by the electron optical properties of the input lens. Consequently we would expect that any differences in the transmission of the lens between the two groups of electrons would manifest themselves by differences in the resolution of the two peaks. The data shown in figure 1 were fitted with a double Gaussian fitting programme (see Bevington and Robinson 1990) and it was shown that both the singlet and triplet peaks had the same energy resolution. Therefore we are confident that the present normalization technique does not suffer from any transmission effects.

3. Results and discussion

Differential cross sections for the excitation of the 3^3P state in magnesium at impact energies of 10 and 20 eV are given in table 1. Using the prescription described above absolute values were assigned from the absolute differential cross sections for the excitation of the 3^1P state of Brunger *et al* (1988). The errors shown are plus and minus one standard deviation. The uncertainty in the normalization constant was obtained by adding in quadrature the uncertainty in the ratio of R_θ, the quoted error in the 3^1P differential cross section of Brunger *et al* (1988) and the statistical error in the scattered intensity of the 3^3P state at the normalization angle. The errors in the cross sections were obtained by adding the error in the normalization constant in quadrature with the statistical errors in the angular distribution at each scattering angle.

The cross sections are shown in figures 2 and 3 where they are compared with the cross sections predicted by the perturbation theory calculation of Avdonina and Amuy'sa

Table 1. Differential cross sections for the excitation of the 3^3P state in magnesium by electrons of 10 and 20 eV.

	Differential cross section (a_0^2 sr^{-1})	
Electron angle θ_e (deg)	$E_0 = 10$ eV	$E_0 = 20$ eV
10	$1.82E+00 \pm 1.34E-01$	$5.59E-01 \pm 3.40E-02$
15	$2.04E+00 \pm 1.57E-01$	$6.12E-01 \pm 3.70E-02$
20	$2.33E+00 \pm 1.67E-01$	$6.63E-01 \pm 4.02E-02$
25	$2.37E+00 \pm 1.35E-01$	$6.66E-01 \pm 4.00E-02$
28	—	$6.56E-01 \pm 3.95E-02$
30	$2.26E+00 \pm 1.16E-01$	$6.45E-01 \pm 3.88E-02$
35	$2.09E+00 \pm 1.42E-01$	$6.17E-01 \pm 3.71E-02$
40	$2.03E+00 \pm 1.14E-01$	$5.57E-01 \pm 3.35E-02$
45	$1.82E+00 \pm 1.03E-01$	$4.63E-01 \pm 2.79E-02$
50	$1.57E+00 \pm 8.03E-02$	$3.50E-01 \pm 2.12E-02$
60	$1.35E+00 \pm 7.05E-02$	$1.70E-01 \pm 1.05E-02$
70	$1.04E+00 \pm 5.98E-02$	$5.65E-02 \pm 3.82E-03$
80	$7.13E-01 \pm 4.05E-02$	$1.78E-02 \pm 2.16E-03$
90	$5.71E-01 \pm 4.27E-02$	$8.93E-03 \pm 2.08E-03$
100	$3.34E-01 \pm 3.21E-02$	$2.07E-02 \pm 2.28E-03$
110	$1.65E-01 \pm 1.47E-02$	$2.62E-02 \pm 2.36E-03$
120	$1.05E-01 \pm 1.27E-02$	$2.54E-02 \pm 2.19E-03$
130	$1.58E-01 \pm 1.20E-02$	$1.72E-02 \pm 1.96E-03$

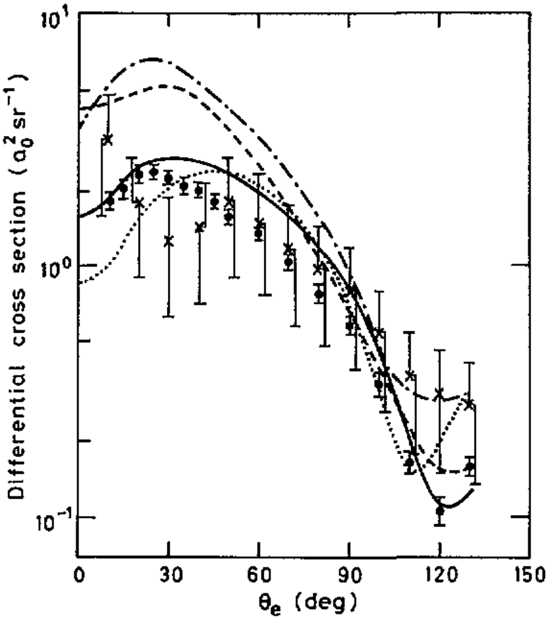

Figure 2. Absolute differential cross sections for the electron excitation of the 3^3P state in magnesium at 10 eV. The present results, ●; are compared with the data of Williams and Trajmar (1978), ×; and with the predictions of Avdonina and Amus'ya (1983), — · —; the CCOM (1989), ——; a six-state CC calculation of McCarthy *et al* (1989), · · · · · ·; and the FOMBT (1990), – – –.

(1983). The present data are also compared with the predictions of the FOMBT calculation

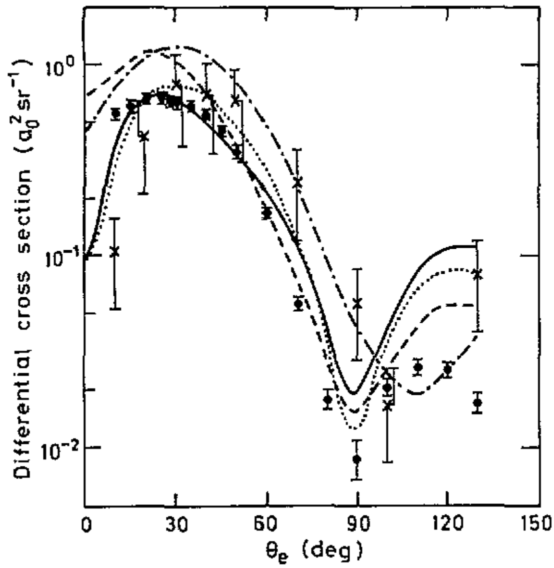

Figure 3. Absolute differential cross sections for the electron excitation of the 3^3P state in magnesium at 20 eV. The present results, ●; are compared with the data of Williams and Trajmar (1978), ×; and with the predictions of Avdonina and Amus'ya (1983), — · —; the CCOM (1989), ——; a six-state CC calculation of McCarthy *et al* (1989), · · · · · ·; and the FOMBT (1990), – – –.

of Meneses *et al* (1990) and with the two most recent coupled channels calculations of McCarthy *et al* (1989); a six state close coupling calculation and a six state close coupling calculation which includes continuum optical potentials (CCOM). The present results are in generally good agreement with the previous measurements of Williams and Trajmar (1978) but the improved accuracy of our measurements permits a more meaningful comparison between theory and experiment.

At an incident energy of 10 eV no theory predicts the differential cross sections over the whole angular range. The perturbation theory calculation of Avdonina and Amuy'sa (1983) predicts the shape of the cross sections at forward angles but the absolute values of the theory here differ by a factor of about three from the present measurement. Although the coupled channels calculations predict a minimum in the cross section at backward angles, the inclusion of the optical potential brings the theory more in line with the experiment. The optical potentials also improve the theory at forward angles but both coupled channel calculations significantly overestimate the cross sections at middle angles. The FOMBT theory also predicts the backward angle miminum correctly but is overestimates the cross section by about a factor of two at forward angles.

At 20 eV all theories, apart from the perturbation theory calculation, successfully predict the minimum at 90°, however all these theories significantly overestimate the cross section at that minimum. These theories also predict a second maximum in the cross section at about 120°. At this energy the benefits of including the optical model in the coupled channels calculation are not as obvious as they were at 10 eV. The FOMBT is in better agreement with the data at 20 eV than at 10 eV but there is still about a factor of two difference between theory and experiment at forward angles.

We note that the recent ten-state calculation of Zhou (1994) produced results for the 3^3P state that were almost identical to those of McCarthy *et al* (1989) at both 10 eV and

Table 2. Integral cross sections (in units of $\pi a_0{}^2$) at 10 and 20 eV impact energies. McCarthy *et al* (1989) refers to their CCOM calculation only.

	Integral cross section (πa_0^2)			
Impact energy E_0 (eV)	Present	Williams and Trajmar (1978)	FOMBT Meneses *et al* (1990)	CCOM McCarthy *et al* (1989)
10	3.2	3.53	4.76	4.31
20	0.56	0.9	0.57	0.69

20 eV. Consequently we do not plot Zhou's results.

The differential cross sections were extrapolated in the range $0° \leqslant \theta < 10°$ and in the range $130° < \theta \leqslant 180°$ by fitting the measured values to a seventh order polynomial. The integral cross sections $Q(E_0)$, are given by

$$Q(E_0) = 2\pi \int_0^\pi \sigma(\theta) \sin\theta \mathrm{d}\theta \tag{6}$$

and are evaluated numerically using Simpson's method. The estimated 3^3P integral cross sections at incident energies of 10 eV and 20 eV are given in table 2 where they are compared with the integral cross sections determined by Williams and Trajmar (1978) and with the theoretical predicitions of the calculations of McCarthy *et al* (1989) and with the FOMBT of Meneses *et al* (1990). We note that given an additional uncertainty associated with the present extrapolation procedure we ascribe the, possibly conservative, error limits on our integral cross sections to be $\pm 20\%$. At both 10 and 20 eV the CCOM theory of McCarthy *et al* (1989) overestimates the total cross section by about 30%. This behaviour is consistent with that found in an earlier application of the model by McCarthy and Mitroy (1989) for the excitation of the 3^1P state. The FOMBT theory on the other hand predicts total cross sections which are in excellent agreement with the present results at 20 eV. This is perhaps fortuitous given the rather poor agreement between this theory and the differential cross sections, as is shown in figure 3. Nevertheless it can be understood by the observation that equation (6) preferentially weights good agreement in the middle angle region because of a factor of $\sin\theta$ in the integrand.

4. Conclusions

Although none of the theories which are compared with the present data provide an adequate description of the differential cross sections for the excitation of the 3^3P state in magnesium, the theory which would seem to offer more chance for improvement is the close coupling calculation of McCarthy and co-workers. The relative failure of this model at middle angles indicates that the treatment of electron exchange in the model is inadequate. This latter observation is consistent with the recent result of Bray *et al* (1994) who have extended their convergent close coupling model to 'two-electron' atoms. In this particular application they found that with a more sophisticated exchange model than that applied earlier by Brunger *et al* (1990), and which was also employed by McCarthy *et al* (1989) and Zhou (1994) in their magnesium studies, excellent agreement was now obtained with experiment (Brunger *et al* 1990, Trajmar 1973) for the electron impact excitation of the 2^3S and 2^3P states of helium. We believe that an extension of the convergent close coupling method to electron impact excitation of the 3^3P state of magnesium might well lead to a similarly satisfactory result to that found for helium.

Acknowledgments

This research was supported in part by a grant from the Australian Research Council. One of us (RKH) acknowledges support from an Australian Post Graduate Research Award.

References

Avdonina N B and Amuy'sa M Y 1983 *Sov. Phys.-Tech. Phys.* **28** 209–13

Bevington P R and Robinson D K 1990 *Data Reduction and Error Analysis for the Physical Sciences* (London: McGraw-Hill)

Bray I, Fursa D V and McCarthy I E 1994 *J. Phys. B: At. Mol. Opt. Phys.* **27** in press

Brunger M J, McCarthy I E, Ratnavelu K, Teubner P J O, Weigold A M, Zhou Y and Allen L J 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** 1325–35

Brunger M J, Riley J L, Scholten R E and Teubner P J O 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 1639–48

Buckman S J, Hammond P, King G C and Read F H 1983 *J. Phys. B: At. Mol. Opt. Phys.* **16** 4219–326

Harting E and Read F H 1976 *Electrostatic Lenses* (London: Elsevier) p 143

Kuhn H G 1969 *Atomic Spectra* (London: Longmans) p 192

McCarthy I E, Ratnavelu K and Zhou Y 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 2597–603

McCarthy I E and Mitroy J D 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 641–54

Meneses G D, Pagan C B and Machado L E 1990 *Phys. Rev.* A **41** 4740–50

Teubner P J O, Riley J L, Brunger M J and Buckman S J 1986 *J. Phys. B: At. Mol. Phys.* **19** 3313–26

Trajmar S 1973 *Phys. Rev.* A **8** 191–203

Williams W and Trajmar S 1978 *J. Phys. B: At. Mol. Phys.* **11** 2021–9

Zhou Y 1994 *PhD Thesis* Flinders University of South Australia (unpublished)