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# Low-energy electron scattering by atomic magnesium

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**Abstract.** The cross sections for low-energy elastic scattering of electrons from the ground state of Mg and excitation cross sections for the $3^1P$ and $3^3P$ states are calculated using the close coupling approximation. Semiempirical wavefunctions are used in the calculation. The results differ greatly from a similar calculation of Van Blerkom and an attempt is made at explaining the difference. From the $T$-matrix elements obtained the polarization of radiation excited by electron impact is calculated for Mg isotopes with a zero nuclear spin.

## 1. Introduction

By now the cross sections for low-energy electron scattering by Mg have been calculated by several authors. Van Blerkom (1970) presented close coupling calculations for the cross sections corresponding to all transitions between the $3^1S$, $3^3P$ and $3^1P$ states. Savchenko (1970) calculated the cross sections for excitation of the fine structure components $3^1P_1$ and $3^3P_{0,1,2}$ using Ochkur approximation. In this paper results of close coupling calculations are presented for the elastic scattering cross sections from the $3^1S$ state and for the excitation cross sections for the $3^1P$ and $3^3P$ states. The results disagree strongly with those of Van Blerkom. In § 3 we shall give one of the possible explanations to this discrepancy based on the analysis of some limiting relations for the cross sections.

## 2. Calculations

The semiempirical wavefunctions we use were calculated by Anderson *et al* (1967) in the following way. A valence electron is regarded as moving in the effective potential which is first calculated by Hartree–Fock method and is then linearly deformed so that the eigenvalue of the Schrödinger equation with this potential coincide with the experimentally determined energy level.

It was assumed when deriving the close coupling equations that a valence shell wavefunction for an excited state could be written as

$$\Psi_i(1, 2) = \frac{1}{2^{1/2}}[\psi_0(1)\psi_i(2) \pm \psi_0(2)\psi_i(1)]$$

where $\psi_0$ is the one-electron ground state wavefunction, and $\psi_i$ is the one-electron function of the p-electron for an excited i-state.

It agrees with the assumption that the s-electron wavefunction is independent of electronic configuration. Under the condition

$$\left(1-\int \psi_0^* \psi_{0i}\, d\tau\right) \ll 1$$

($\psi_{0i}$ is the s-electron function for an i atomic state) which is satisfied in our case, we can show that such a substitution will not introduce a large error. In addition according to the semiempirical method expressions of the form

$$\int \Psi_i^* H_a \Psi_i\, d\tau - \int \Psi_0^* H_a \Psi_0\, d\tau$$

($H_a$ is the atomic hamiltonian) were replaced by $\epsilon_i - \epsilon_0$, where $\epsilon_i$ is the experimentally observed ionization potential. As a result of this substitution the inelastic process thresholds became equal to the experimentally observed ones.

The equations obtained were solved only for the case of $S = \frac{1}{2}$, $\pi = 0$, because we did not calculate the cross sections for transitions between the excited states. The equations were solved following Marriot's (1958) noniteration scheme. Outward and inward integration was performed by Miln's prediction and correction method. At large distances the asymptotic expansions of Burke and Schey (1962) were used. In the calculation of the cross sections 4 to 8 partial waves were taken into account, exchange being included at $L \leqslant 3$. At some points with sufficiently large $L$ and small $E$ we used the formula of O'Malley *et al* (1961) for the phase shift

$$\tan \delta_L = \frac{\pi \alpha k^2}{(2L-1)(2L+1)(2L+3)} \tag{1}$$

where $\alpha$ is the atomic polarizability.

## 3. Results

The calculated cross sections are presented in figures 1 and 2 where comparison is also made with Van Blerkom's results. The maximum of the cross section for elastic scattering in the region of $E \approx 0{\cdot}19$ Ryd is due to the fact that the $L = 2$ phase shift passes through $\pi/2$ (see figure 3). However, other resonances were not found in the calculation. They may appear in more thorough calculations, ours being performed with a large energy step.

Some values of the partial wave cross sections are given in tables 1, 2 and 3.

Superficially, the large discrepancy between the results of our calculation and that of Van Blerkom is surprising. A possible cause of this discrepancy can be indicated by the following reasoning.

If $L \geqslant 2$, then at low energies the scattering phase growth obeys the law (1). (At $L = 1$ the region of validity of the law is very small.) As only one state is included which is coupled through a long-range potential with the ground state, the polarizability $\alpha$ is given by the formula

$$\alpha = \frac{f}{(\epsilon_1 - \epsilon_0)^2}, \tag{2}$$

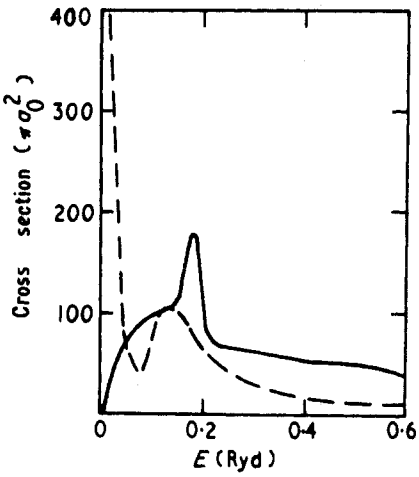


**Figure 1.** Total cross sections for elastic scattering from the ground state; ——— Van Blerkom's results.

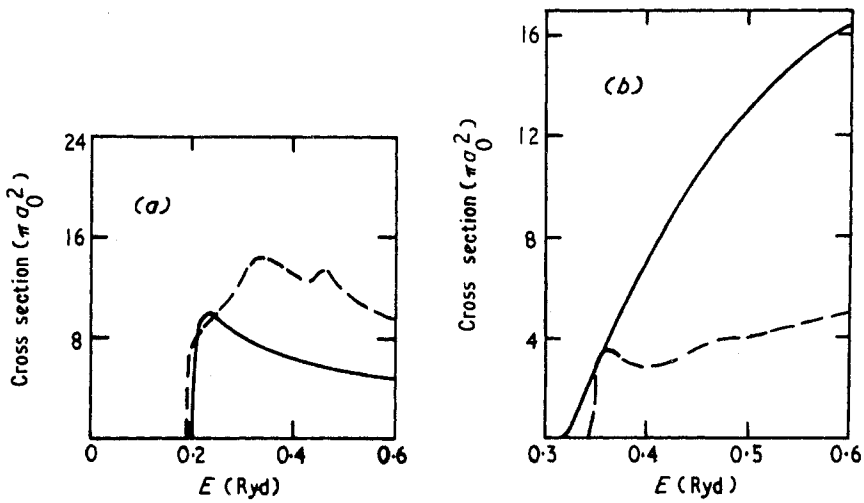


**Figure 2.** Total cross sections for excitation of (*a*) the $3^3P$ state (*b*) the $3^1P$ state; ——— Van Blerkom's results.

where $f$ is the oscillator strength of the $3^1S$–$3^1P$ transition and $\epsilon_0$ and $\epsilon_1$ are the corresponding energy levels. Calculation using semiempirical functions gives $f = 2{\cdot}12$ (see Anderson *et al* (1967)). If this value is substituted into (2) and (1), we obtain a formula which at small $k^2$ agrees with the cross sections we obtained for $L \geqslant 2$ (see table 1). However, the partial cross sections for $L \geqslant 2$ in this region calculated by Van Blerkom are less than ours by a factor of 20. Since at small $\delta_L$ the partial cross section is proportional to $\mathrm{tg}^2\,\delta_L$, it implies that Van Blerkom's results can be explained if one assumes that the wavefunctions she uses give an oscillator strength of about $20^{1/2} \approx 4{\cdot}5$ times less than ours. However, no theoretical calculation, in particular that of Zare (1967)

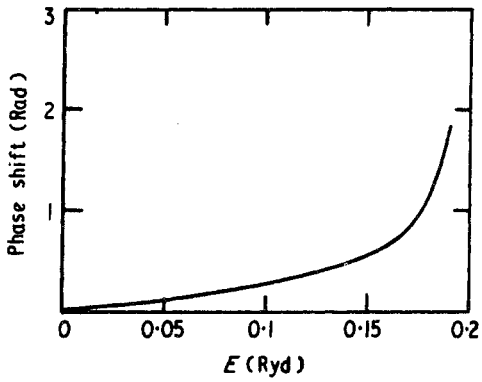


**Figure 3.** $L = 2$ phase shift of elastic scattering from the ground state.

**Table 1.** $3^1S$–$3^1S$ cross section ($\pi a_0^2$)

| $E$ (Ryd) | $L = 0$ | $L = 1$ | $L = 2$ | $L = 3$ | $L = 4$ | $L = 5$ | $L = 6$ | $L = 7$ | Total |
|---|---|---|---|---|---|---|---|---|---|
| 0·01 | 4·90 | 1·92 | 1·78 | 0·094 | | | | | 8·61 |
| 0·05 | 25·3 | 39·8 | 5·97 | 0·31 | 0·23 | | | | 71·4 |
| 0·1 | 26·6 | 54·5 | 14·7 | 0·60 | 0·44 | 0·18 | | | 97·0 |
| 0·185 | 20·7 | 49·6 | 104·7 | 2·56 | 0·80 | 0·32 | | | 179 |
| 0·3 | 12·8 | 33·3 | 7·67 | 6·00 | 1·42 | 0·57 | 0·24 | | 62·1 |
| 0·4 | 8·39 | 22·6 | 9·70 | 9·31 | 2·31 | 0·82 | 0·38 | | 53·6 |
| 0·5 | 5·49 | 17·7 | 9·68 | 6·89 | 3·19 | 1·08 | 0·43 | 0·20 | 44·8 |
| 0·6 | 3·61 | 13·8 | 9·38 | 4·99 | 3·54 | 1·38 | 0·56 | 0·26 | 37·6 |

**Table 2.** $3^1S$–$3^3P$ cross section ($\pi a_0^2$)

| $E$ (Ryd) | $L = 0$ | $L = 1$ | $L = 2$ | $L = 3$ | Total |
|---|---|---|---|---|---|
| 0·25 | 0·074 | 2·41 | 7·08 | | 9·56 |
| 0·3 | 0·12 | 2·61 | 5·59 | 0·068 | 8·39 |
| 0·4 | 0·13 | 2·21 | 3·58 | 0·67 | 6·59 |
| 0·5 | 0·11 | 1·84 | 2·66 | 0·94 | 5·55 |
| 0·6 | 0·086 | 1·52 | 2·04 | 0·97 | 4·62 |

**Table 3.** $3^1S$–$3^1P$ cross section ($\pi a_0^2$)

| $E$ (Ryd) | $L = 0$ | $L = 1$ | $L = 2$ | $L = 3$ | $L = 4$ | $L = 5$ | $L = 6$ | $L = 7$ | Total |
|---|---|---|---|---|---|---|---|---|---|
| 0·4 | 0·0019 | 1·86 | 1·00 | 3·67 | 0·38 | | | | 6·91 |
| 0·5 | 0·0043 | 1·45 | 1·73 | 6·54 | 2·04 | 0·77 | 0·30 | 0·11 | 13·0 |
| 0·6 | 0·0087 | 1·28 | 2·06 | 6·17 | 3·68 | 1·79 | 0·88 | 0·43 | 16·5 |

gives such a small value of the oscillator strength for Mg. Hence, it seems that our results are more probable.

The above considerations refer to the case of small $k^2$ and $L \geqslant 2$. However, as is seen from a comparison of Van Blerkom's results with data in table 1 of the present

paper, a strong discrepancy in the partial cross sections for elastic scattering is observed in the other regions too, except for the region $L = 0, k^2 > 0{\cdot}01$ Ryd. It might be (though not necessarily so) that these discrepancies, as well as those in the excitation cross sections are due to the same cause.

That Van Blerkom's oscillator strength of the resonance transition is small can be concluded from other reasoning. We calculated the cross sections for excitation of the $3^1P$ state as Van Blerkom did, by Milford's formula (1960) which is a variant of Bethe approximation. The values of the cross sections obtained are about four times those of Van Blerkom calculated by the same formula. As this formula involves the first power oscillator strength we arive at the same conclusion.

Here it should be noted that in our case the values of cross sections for excitation of the $3^1P$ state seem to be somewhat too large, because the value of the oscillator strength obtained from our functions exceeds both the experimental findings and the results of most other theoretical calculations. The error can exceed 25–30 %.

Comparison of our results with those of Savchenko (1970) is difficult because his cross sections depend greatly on the choice of wavefunctions. It can be noted, however, that the cross sections for excitation of the $3^1P$ state calculated using Bates and Damgaard functions are very close to ours. As far as the cross sections for excitation of the $3^3P$ state are concerned, there is no agreement. This can be explained by the fact that excitation of the $3^3P$ state is due to the exchange interaction (spin–orbit interaction taken into account by Savchenko plays a minor role for Mg) and its inclusion in Ochkur approximation may be insufficient.

## 4. Polarization of radiation

Starting with the $T$-matrix for excitation of the $^1P$ and $^3P$ states we calculated the polarization of the radiation excited by electron impact. For Mg atoms which nucleus are the $Mg^{24}$ and $Mg^{26}$ isotopes there is no hyperfine structure separation and fine structure separation is large compared with the line-widths. Then following Percival and Seaton (1958) for the photons emitted perpendicular to the incident electron beam the polarization is

$$P = \frac{1-x}{1+x} \qquad \text{for the } {}^1P\text{–}{}^1S \text{ transition}$$

$$P = \frac{15(1-x)}{41+67x} \qquad \text{for the } {}^3P\text{–}{}^1S \text{ transition}$$

where $x = \sigma_1/\sigma_0$ and $\sigma_1, \sigma_0$ are the cross sections for excitation of the states with magnetic quantum numbers 1 and 0, respectively. Of the stable isotopes $Mg^{25}$ with a nuclear spin $\frac{5}{2}$ remains. To calculate the polarization of radiation corresponding to it one should know the magnitude of hyperfine structure separation. In this paper we confined ourselves to $Mg^{24}$ and $Mg^{26}$ calculations, the more so that their isotope abundance in normal mixture accounts for 89·9 %.

The $\sigma_0$ and $\sigma_1$ cross sections were calculated by the formula given by Burke *et al* (1963) taking into account what was said in Burke *et al* (1969) paper about the additional factor $i^{L-L'}$.

The percentage polarization of radiation emitted from the $3^1P$ state at incident electron energies 0·35, 0·4, 0·45, 0·5, 0·6 Ryd accounted for 91, 64, 65, 60, 53 %, respectively. Polarization of radiation emitted from the $3^3P$ state changes little in the range 0·35–0·6 Ryd within 20–25 %.

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