Calculation of Cross Sections for Elastic Scattering of Electrons at Intermediate Energies by a Magnesium Atom

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We have obtained differential and integral cross sections for elastic scattering of electrons by magnesium atom at 10 – 100 eV using a complex, local, energy-dependent, spherically-symmetric optical potential incorporating a modified semi-classical exchange potential. The results have been compared with available theoretical and experimental results. The present results are in good agreement with recent experimental results at electron impact energies $E \geq 40$ eV and are in qualitative agreement at lower energies. The results indicate the reliability of the modified exchange potential at higher energies in the intermediate energy range.

1. Introduction

The availability of accurate differential and integral cross section experimental data on electron scattering by atoms and molecules provides strong impetus for development of theoretical methods for description of scattering processes. In elastic electron-atom and electron-molecule scattering substantial effort has been directed towards formulation of a suitable optical potential that yields results, which are in close agreement with measured results (Hein et al. [1], de Souza et al. [2], Blanco and Garcia, [3]). One aspect of the optical potential that has attracted particular attention is the non-local exchange potential. Furness and McCarthy [4] approximated the potential to a local semi-classical exchange potential, which was later modified by Gianturco and Scialla [5] using a free-electron gas model to describe the bound electrons. In this paper, we have further modified the semi-classical potential using the Hartree-Slater approximation to the Hartree-Fock equations and applied this new exchange potential to the problem of elastic scattering of electrons by magnesium atom.

Several theoretical and experimental results for elastic scattering of electrons by magnesium atom at intermediate energies have been reported (Predojevic et al. [6]). The optical potential calculations so far reported include the results of Khare et al. [7] and the results of Yousif and Lennart [8]. Both calculations used real optical potentials, which did not account for the loss of flux into inelastic channels at intermediate energies. In the present calculation, the static potential and the proposed exchange potential are calculated using the Hartree-Fock wavefunctions of Bunge et al. [9] for the magnesium ground state. For the polarization potential, we have used the energy-dependent potential of Valone et al. [10] incorporating the adiabatic potential of Eades et al. [11] and to account for excitation and ionization of the magnesium atom by the impinging electrons the quasifree absorption potential (version 2) of Staszewska et al. [12] has been applied. The present results are compared with the recent experimental results of Predojevic et al. [6], the earlier measured results of Williams and Trajmar [13], the optical potential results of Khare et al. [7], and the five-state close-coupling results of Mitroy and McCarthy [14].

2. Theory

In the optical potential method, the many-body electron-atom elastic scattering problem is reduced to a one-body problem in which the wave function of the scattering electron is governed by the radial equation

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + 2\left(E - V_{opt}\right)\right)u_l(r) = 0 \qquad (1)$$

Where, E is the energy of the incident electron (in Hartree atomic units) and V_{opt} is the complex non-local optical potential usually approximated to a potential of the form

$$V_{opt} = V_{st} + V_{ex} + V_{pol} + iV_{abs} \qquad (2)$$

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In Eqn. (2), V_{st} is the static potential, V_{ex} is the exchange potential, V_{pol} is the polarization potential and V_{abs} is the absorption potential. The static potential is given in terms of the radial wave functions P_{nl} of the target atom by

$$V_{st}(r) = -\frac{Z}{r} + \sum_{nl} N_{nl} \int_0^\infty dr' \frac{P_{nl}^2(r')}{r_>} \quad (3)$$

Where, Z is the atomic number of the atom, N_{nl} is the occupation number of the atomic orbitals and $r_>$ denotes the greater of r and r'.

The non-local exchange potential is given according to Furness and McCarthy [4] as

$$V_{ex}\varphi_o(\vec{r}) = -\sum_i \int d^3r' \varphi_i^*(\vec{r}') \frac{1}{|\vec{r}' - \vec{r}|} \varphi_o(\vec{r}') \varphi_i(\vec{r}) \quad (4)$$

In this equation, φ_i is the wave function of the i[th] bound electron and φ_o is the wave function of the continuum electron defined, respectively, as

$$\varphi_i(\vec{r}) = \frac{1}{r} P_{nl}(r) Y_{lm}(\hat{r}) \chi_\mu(\sigma) \quad (5)$$

$$\varphi_o(\vec{r}) = u_l(r) Y_{lm}(\hat{r}) \chi(\sigma) \quad (6)$$

Following Gianturco and Scialla [5], we approximate the integral in Eqn. (4) by

$$\int d^3r' \varphi_i^*(\vec{r}') \frac{1}{|\vec{r}' - \vec{r}|} \varphi_o(\vec{r}') \approx -\frac{4\pi}{\nabla^2 + \nabla_i^2} \varphi_i^*(\vec{r}) \varphi_o(\vec{r}) \quad (7)$$

The operators ∇^2 and ∇_i^2 act on the continuum and atomic wave functions, respectively, according to the following equations

$$\nabla^2 \varphi_o(\vec{r}) = -2(E - V_{st} - V_{ex}) \varphi_o(\vec{r}) \quad (8)$$

$$\nabla_i^2 \varphi_i^*(\vec{r}) = -2(\varepsilon_{nl} - V_{st} - V_x) \varphi_i^*(\vec{r}) \quad (9)$$

In Eqn. (9), ε_{nl} is the binding energy of the bound electrons in the P_{nl} orbital and V_x is the local Hartree-Slater approximation to the Hartree-Fock exchange potential given by Cowan [15] in terms of the electron charge density $\rho(r)$ as

$$V_x = -\frac{3}{4}\left(\frac{24\rho}{\pi}\right)^{1/3} \quad (10)$$

Using Eqns. (7)-(9) in Eqn. (4) and carrying out summations over the spin-orbitals yields the following local exchange potential

$$V_{ex}(r, E) = -\frac{1}{4r^2} \sum_{nl} \frac{N_{nl} P_{nl}^2(r)}{T_{loc} + (\varepsilon_{nl} - V_{st} - V_x)} \quad (11)$$

Where, $T_{loc} = E - V_{st} - V_{ex}$, is the local kinetic energy of the incident electron in the vicinity of the target atom. In our calculation, this exchange potential is determined iteratively.

The polarization potential, which in principle involves an infinite sum over excited target states, has been taken in the present calculation as the semi-classical approximation of Valone et al. [10] is given by

$$V_{pol}(r, E) = V^{ad} / (1 + T_{loc}/\Delta) \quad (12)$$

In this equation, Δ is the mean excitation energy of the magnesium atom and V^{ad} is the energy-independent part of the polarization potential that we have taken as the potential of Eades et al. [11]. For the absorption potential, we have taken the quasi-free absorption potential (version 2) proposed by Staszewska et al. [12] and given in terms of the local velocity of the scattering electron υ_{loc} and the mean binary collision cross section $\overline{\sigma}_b$ as

$$V_{abs} = -\frac{1}{2} \upsilon_{loc} \rho(r) \overline{\sigma}_b \quad (13)$$

With these approximations to the optical potential, Eqn. (1) is solved numerically using the Numerov method subject to the following boundary conditions

$$u_l(r = 0) = 0 \quad (14a)$$

$$\lim_{r \to \infty} u_l(r) = a_l (f_l(kr) - \tan \delta_l g_l(kr)) \quad (14b)$$

In Eqn. (14b), f_l and n_l are the Ricatti-Bessel functions and δ_l is the complex phase shift corresponding to the radial wave function u_l. According to Schiff [16], the scattering amplitude

$f(\theta)$ is given in terms of the phase shifts and the Legendre Polynomials P_l by

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left(e^{2i\delta_l}-1\right)P_l(\cos\theta) \qquad (15)$$

The differential cross section is calculated from the scattering amplitude by

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \qquad (16)$$

Finally, the integral (elastic + inelastic) cross section is determined using the equation

$$\sigma_I = \frac{2\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[1-\mathrm{Re}(S_l)] \qquad (17)$$

Where, $S_l = e^{2i\delta_l}$, is an element of the S-matrix.

3. Results and Discussion

The present differential cross section results, obtained using a complex potential for elastic scattering of electrons by a magnesium atom at 10, 15, 20, 40, 60, 80 and 100 eV, are given in Table 1. In Fig. 1 the present DCS results are compared with the results of Predojevic et al. [6], Khare et al. [7], Williams and Trajmar [13], and the results of Mitroy and McCarthy [14]. For better comparison with the results of Khare et al. [7], we have also presented results without the absorption potential.

In Fig. 1(a), the present results at 10 eV are lower than the results of Khare et al. [7] for all scattering angles. The difference is not due to inclusion of an absorption potential in our calculation since the results with and without absorption are virtually identical, as can be seen in the figure. Rather, it can be attributed to the exchange and polarization potentials used in our calculation. The present results are in close agreement with the results of Mitroy and McCarthy [14] at scattering angles $\leq 50^o$ but differ appreciably at larger angles. Similarly good agreement between the present results and the experimental results of Williams and Trajmar [13] is restricted to scattering angles $\leq 50^o$. Our results are in good agreement with the experimental results of Predojevic et al. [6] at low scattering angles and at large angles. The present calculation predicts two minima at $\theta = 60^o$ and $\theta = 150^o$. The first minimum coincides with the position of the minimum in the results of Predojevic et al. [6].

In Fig. 1(b), the present calculation predicts two minima at $\theta = 50^o$ and $\theta = 140^o$ in the differential cross sections at 15 eV. The position of the second minimum coincides with the minimum in the results of Predojevic et al. [6] but the minimum is less pronounced in our results. The effect of the absorption potential in lowering the differential cross section is particularly significant near the first minimum.

At 20 eV, our DCS calculated with and without absorption are lower than those of Khare et al. [7] at virtually all scattering angles. The present results are close to the results of Mitroy and McCarthy [14] up to $\theta = 50^o$ but are lower than the results of Williams and Trajmar [13] over this range of scattering angles. Our results have minima at $\theta = 50^o$ and $\theta = 130$ with the positions of these minima coinciding with those in the experimental results of Predojevic et al. [6].

Our calculation with the absorption potential yields results at 40 eV in very good quantitative agreement with the results of Predojevic et al. [6] over all scattering angles. The agreement between our DCS and the experimental results of Williams and Trajmar [13] is good only up to $\theta = 40^o$ with the present results being higher than these measured results at larger scattering angles. Our results without absorption are lower than the results of Khare et al. [7] for angles $\theta < 20^o$ but are in very good agreement at larger angles.

Table 1: Differential cross sections (in $a_o^{\,2} sr^{-1}$) for elastic electron scattering by Mg atom.

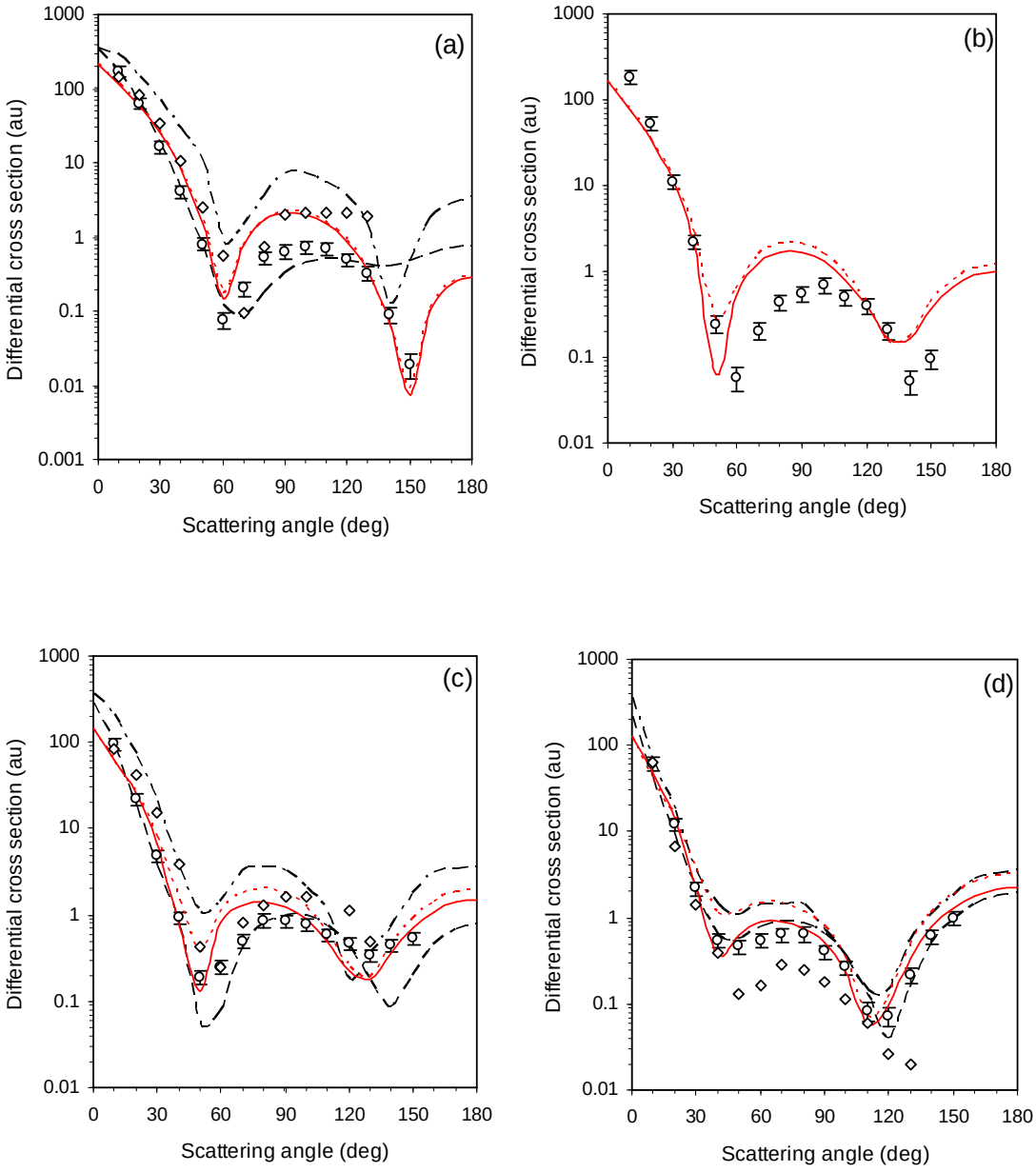
Differential cross section							
Angle (deg)	10 eV	15 eV	20 eV	40 eV	60 eV	80 eV	100 eV
0	2.10E+02	1.63E+02	1.42E+02	1.30E+02	1.37E+02	1.46E+02	1.56E+02
10	1.13E+02	7.67E+01	6.24E+01	4.75E+01	4.19E+01	3.80E+01	3.43E+01
20	5.82E+01	3.45E+01	2.52E+01	1.39E+01	9.70E+00	7.38E+00	5.88E+00
30	2.55E+01	1.17E+01	6.77E+00	2.27E+00	1.64E+00	1.52E+00	1.52E+00
40	8.40E+00	2.24E+00	7.34E-01	3.66E-01	6.52E-01	7.79E-01	8.01E-01
50	1.55E+00	6.41E-02	1.32E-01	6.23E-01	7.57E-01	7.28E-01	6.29E-01
60	1.48E-01	5.22E-01	8.01E-01	8.97E-01	7.74E-01	6.25E-01	4.65E-01
70	7.59E-01	1.28E+00	1.27E+00	8.82E-01	5.95E-01	3.97E-01	2.44E-01
80	1.65E+00	1.68E+00	1.39E+00	7.38E-01	4.03E-01	2.21E-01	1.19E-01
90	2.12E+00	1.67E+00	1.24E+00	5.10E-01	2.16E-01	9.26E-02	4.35E-02
100	2.02E+00	1.31E+00	8.83E-01	2.35E-01	5.00E-02	6.61E-03	8.37E-03
110	1.52E+00	8.11E-01	4.86E-01	6.04E-02	8.27E-03	3.39E-02	6.19E-02
120	8.93E-01	3.90E-01	2.27E-01	9.35E-02	1.31E-01	1.67E-01	1.73E-01
130	3.67E-01	1.63E-01	1.83E-01	3.44E-01	4.04E-01	3.92E-01	3.32E-01
140	6.62E-02	1.66E-01	3.57E-01	7.71E-01	8.01E-01	7.09E-01	5.67E-01
150	7.49E-03	3.68E-01	7.01E-01	1.29E+00	1.24E+00	1.04E+00	8.04E-01
160	1.05E-01	6.65E-01	1.10E+00	1.78E+00	1.62E+00	1.30E+00	9.58E-01
170	2.34E-01	9.12E-01	1.41E+00	2.13E+00	1.89E+00	1.48E+00	1.07E+00
180	2.93E-01	9.90E-01	1.50E+00	2.26E+00	2.03E+00	1.66E+00	1.26E+00

Fig. 1(e) shows that the present results with absorption are in very good agreement with the measured results of Predojevic et al. [6] at 60 eV. The situation is similar at 80 eV but our DCS at this energy have a minimum at $\theta = 100^o$ while the results of Predojevic et al. [6] have a minimum at $\theta = 110^o$.

At 100 eV, Fig. 1(g) shows an excellent agreement between the present results with absorption and the results of Predojevic et al. [6] at scattering angles up to $\theta = 100^o$. However, at larger scattering angles our results are higher than the measured results. Our calculation without the absorption potential yields DCS results that are in close agreement with the calculated results of

Mitroy and McCarthy [14] and of Khare et al. [7] at all scattering angles.

In Table 2, the present integral cross sections for elastic scattering of electrons by magnesium at 10 – 100 eV, obtained using a complex optical potential, are given. Other calculated and measured results are also given for comparison. Our ICS results, with and without absorption, are also compared with other calculated and measured results in Fig. 2. The present results are lower than the results of Khare et al. [7] at low energies but are close at 100 eV. The results with absorption are in agreement with the result of Mitroy and McCarthy [14] at all energies considered. There is a close agreement with the results of Williams and Trajmar [13] at 40 eV but our results are lower at 10 and 20 eV. The present results with absorption are in agreement with the experimental results of Predojevic et al. [6] at all incident energies considered apart from at 15 eV.



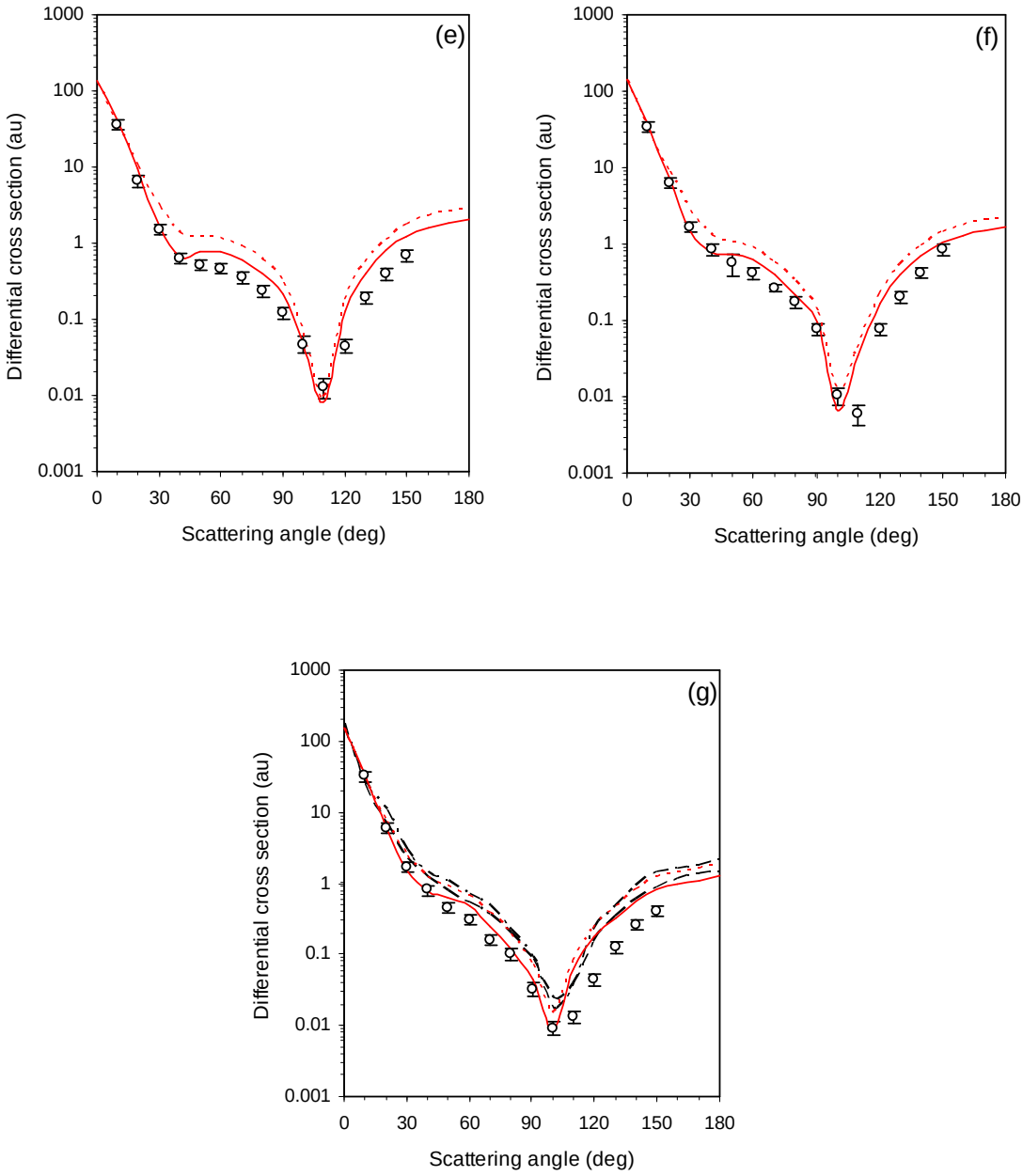


Fig.1: Differential cross sections for elastic scattering of electrons by a magnesium atom at (a) 10 eV (b) 15 eV (c) 20 eV (d) 40 eV(e) 60 eV (f) 80 eV and (g) 100 eV. Theory: full curve, present results with absorption; short-dashed curve, present results without absorption; long-dashed curve, Mitroy and McCarthy [14]; chain curve, Khare et al. [7]. Experiment: circles, Predojevic et al. [6]; diamonds, Williams and Trajmar [13].

Table 2: Integral cross sections (in a_o^2) for electron-Mg elastic scattering.

Theoretical results				Experimental data	
Energy (eV)	Present	Khare et al. [7]	Mitroy and McCarthy [14]	Predojevic et al. [7]	Williams and Trajmar [13]
10	77.75	198.70	79.12	81.77	103.56
15	46.83			73.56	
20	35.73	104.80	37.73	41.78	57.14
40	24.03	35.55	23.69	28.10	23.57
60	19.94			16.53	
80	17.25			16.07	
100	14.97	17.17	15.70	14.32	

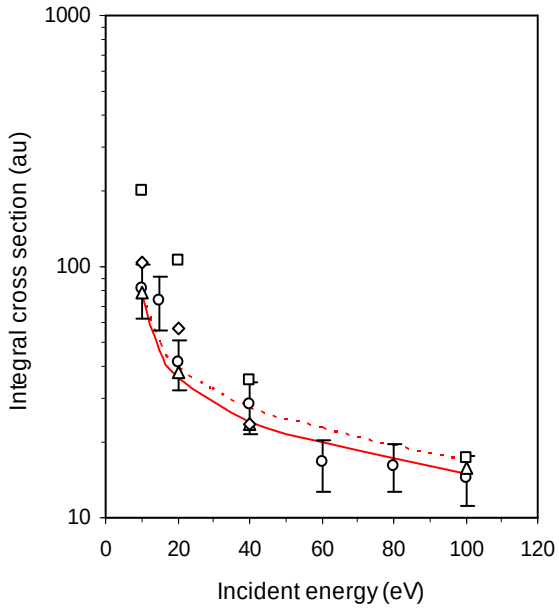


Fig.2: Integral cross sections for elastic scattering of electrons by a magnesium atom at 10 – 100 eV. Theory: full curve, present results with absorption; short-dashed curve, present results without absorption; triangles, Mitroy and McCarthy [14]; squares, Khare et al. [7]. Experiment: circles, Predojevic et al. [6]; diamonds, Williams and Trajmar [13].

4. Conclusions

We have calculated differential and integral cross sections for elastic scattering of electrons by magnesium atom at intermediate energies using a complex optical potential. For the exchange potential, a modified semi-classical potential has been applied. The present DCS are in good qualitative agreement with recent experimental results of Predojevic et al. [6] at $E \le 20$ eV and are in good quantitative agreement with the measured results at higher energies. Our DCS are also in close agreement with the results of Mitroy and McCarthy [13] at small scattering angles at all energies considered. The integral cross sections obtained in our study are within the experimental errors in the results of Predojevic et al. [6] at all energies apart from at $E = 15$ eV where the calculated integral cross section is lower. Our results are also in good quantitative agreement with the results of Mitroy and McCarthy [13] at all electron impact energies. Inclusion of the absorption potential in the optical potential has led to better agreement with measured results but has negligible effect at $E = 10$ eV.

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