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A Numerical Calculation for Electron Impact Excitation of Copper

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The scattering of electrons by atomic copper has been studied using Born approximation and the concept of the generalized oscillator strength (GOS). Differential and total cross-sections for the excitation of the $3d^{10}\ 4p^2$ P state are calculated at incident energies of 100 eV and are compared with other available experimental and theoretical data. The agreement between our calculation for the differential cross-section and the available experimental results is fairly good at the forward angles, while the agreement at large angles is poor. The calculated total cross-sections are compared with the experimental data and those predicted by several theories. It is found that our calculation for the total cross-sections are in a good agreement with the close coupling calculation of Msezane and Henry (1986a, *Physical Review A* **33**, 1631) for incident energies greater than 20 eV. The integrated cross-section measurements of Ismail and Teubner (1995, *Journal of Physics B: Atomic, Molecular and Optical Physics* **28**, 4164) are in good agreement with the present calculation.

KEY WORDS: electron impact excitation; copper.

1. INTRODUCTION

Since the early experiment of Franck and Hertz (1914), the interaction of electrons with atoms has played a fundamental role in the development of atomic physics. Electron scattering from atoms still occupies physicists who seek a description of this fundamental problem. Apart from the importance of cross-section calculation for electron scattering from atoms to diverse fields of physics such as astrophysics, plasma physics, gaseous discharges, and laser physics, the electron scattering problem is of interest from a fundamental point of view. It is known that the electrons and atoms interact through the Coulomb interaction and the scattering process can be described exactly by Schrodinger equation. The solution

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of this equation is impeded by the infinite range of the Coulomb force and by the many body nature of the problem. Consequently scattering theory has been dominated by the many approximations, which have been applied to make the problem more tractable. It is generally acknowledged that the simplest case is electron scattering from atomic hydrogen since the wave functions of the target Hamiltonian are known exactly. Moreover, the calculations of theorists were concentrated on electron scattering from sodium where although the description of the target atom is more difficult than in atomic hydrogen, the scattering problems thought to be simplified by the strong coupling between the ground 3^2S state and the final state.

Electron scattering from copper however is neither easy from the target point of view nor from the scattering point of view. Thus, we conclude that a definitive theoretical description that covers a wide energy range will be difficult to develop. Nevertheless, theories for the excitation of the $3d^{10}4p\ ^2P$ state in copper have appeared in the literature for many years. The reason for this interest is that cross-sections for the excitation of this state are directly relevant to an understanding of the copper vapor laser. The first three states of the copper atom are the ground state with configuration $3d^{10}\ 4s\ ^2S$, $3d^9\ 4s^2\ ^2D$ state, and $3d^{10}4p\ ^2P$ state. Excitation of the P state by electrons is favored on angular momentum grounds over the D-state excitation; consequently, a population inversion can be established between the P and D states, the system can be made to lase at 510.6 and 578.2 nm. Knowledge of the cross-sections for the excitation of these states is clearly relevant to the understanding of the copper vapor laser.

In the present calculations, we confine our attention to the population of the upper ^2P laser level. There are already experimental and theoretical results available, for example Williams and Trajmar (1974), Trajmar *et al.* (1977), Msezane and Henry (1986a,b), Scheibner *et al.* (1987), Pangantiwar and Srivastava (1988), Ismail and Teubner (1995), Madison *et al.* (1998), and more recently Ismail (2003) have reported electron coincidence results for copper. However, at the intermediate energies of 6–100 eV, the available experimental results for differential cross-sections for the excitation of the 4p ^2P state neither agrees in satisfactory manner with each other (Ismail and Teubner, 1995, nor with the available calculations.

Integral cross-section measurements for the 4p ^2P state in the energy range from 10 to 75 eV have been reported by Aleksakhin *et al.* (1979), Borozdin *et al.* (1977), and by Ismail and Teubner (1995) for the energies 20–100 eV. For the total cross-sections, the available calculations are varied with each other and with the available measurements except with those of the close-coupling (cc) calculations of Msezane and Henry (1986a) and the measurements of Ismail and Teubner (1995). Therefore, it is obvious that further theoretical effort needs to be devoted in order to clear these disagreements. However in the intermediate energy region of 40–100 eV, Born calculation has proved to be a useful model for electron atom excitation.

In this paper we reconsider the 4s → 4p excitation by electron impact in copper and report the calculations employing Born calculation and the generalized oscillator strength (GOS) concept at incident electron energies of 6, 10, 20, 40, 60, 80, and 100 eV.

The theoretical techniques used in this study are described in Section 2. The results are presented and discussed in Section 3 and the conclusions are given in Section 4.

2. THEORY

When an electron interacts with atom, the basic interaction that takes place is the Coulomb interaction. The interaction can be totally described by Schrodinger equation. The standard procedure of solving the Schodinger equation is to expand the total wavefunction in terms of eigenfunctions of the target Hamiltonian (Mott and Massey, 1965).

An infinite set of coupled second order differential equations is formed such that

$$\left[\nabla^2 + K_n^2\right] F_n\,(r_1) = \sum_m U_{nm}(r) F_m(r) \tag{1}$$

In the Born approximation, this can be reduced to

$$\left[\nabla^2 + K_n^2\right] F_n\,(r_1) = U_{n0}\, e^{iK_0 r_1} \tag{2}$$

and the differential cross-section is related to the square of the Born scattering amplitude, so that,

$$\frac{d\sigma(\theta)}{d\Omega_e} = \frac{K_n}{K_0} |\, f_n(\theta)|^2 \tag{3}$$

and in terms of the GOS for a transition, the differential cross-section can be expressed as

$$\sigma(\theta) = \frac{2K_n\, f(K)}{W K_0 K^2} \tag{4}$$

where W is the binding energy of the excited state and K' is the momentum transfer between the incident momentum K_0 and the final momentum K_n for the electron scatterd through an angle θ, that is

$$\vec{K} = \vec{K}_0 - \vec{K}_n \tag{5}$$

$$f(K) = f_0 - AK^2 + BK^4 \tag{6}$$

This is valid for small K^2 (Brunger *et al.*, 1988), where $f(k)$ will be approaching the optical oscillator strength $f_0 = 0.645$ (Hannaford and McDonald, 1978), $A = 4.8$ and $B = 21.2$ (Ismail and Teubner, 1995).

The GOS concept is based on Born approximation and the use of this technique depends heavily on the validity of this approximation in the energy range under consideration.

2.1. Integral Cross-Sections

Integral cross-sections Q for the excitation of the $3d^{10}\,4p\,^2P$ state were derived by integrating the deferential cross-section over the scattering angle using

$$Q = 2\pi \int_0^{2\pi} \sigma(\theta)\, \sin\theta\, d\theta \tag{7}$$

3. RESULTS AND DISCUSSION

3.1. Integral Cross-Sections

The integral cross-sections for the excitation of the $3d^{10}\,4p\,^2P$ state calculated using Eqs. (4), (6), and (7) are given in Table I and are displayed in Fig. 1 together with the various calculations and measurements.

The differential cross-sections at the energy range between 20 and 100 eV studied in the present calculations were very strongly peaked in the forward direction. At 20 eV, 85% of the integral comes from the angular range less than 20° whilst at 100 eV 98% of the integral came from the range between 0 and 15°. Since the validity of Born approximation is restricted to small scattering angles, where the incident electron is perturbed slightly by the target, our present calculation is restricted only to small scattering angles.

It is clear that there is a good agreement between the present calculations of the total cross-section and the predictions of the coupled channels theory of Msezane and Henry (1986a) and also in an excellent agreement with the measurements of Ismail and Teubner (1995) at energies grater than 40 eV, as shown in Fig. 1. The present calculations disagree with the previous results of Aleksakhin *et al.* (1979) which are clearly too large. In Fig. 1 we can see also Born approximation calculations by Winter (1977). Peterkop and Liepinsh (1979), and Pangantiwar and Srivastava (1988). They differ from each other and from the present calculation. The difference between the calculations can be attributed to the different descriptions of the target wavefunctions used in the theories. For example the wavefunction used by Peterkop and Liepinsh (1979) gave 0.92 for the optical oscillator strength Whilst that was used by Winter (1977) gave 1.257. The

Table I. Integral Cross-Sections for the Excitation of the $3d^{10}\,4p\,^2P$ State in Copper

E (eV)	6	10	20	40	60	80	100
Q (Πa^2)	27.9	17.8	12.7	9.3	6.9	5.3	4.4

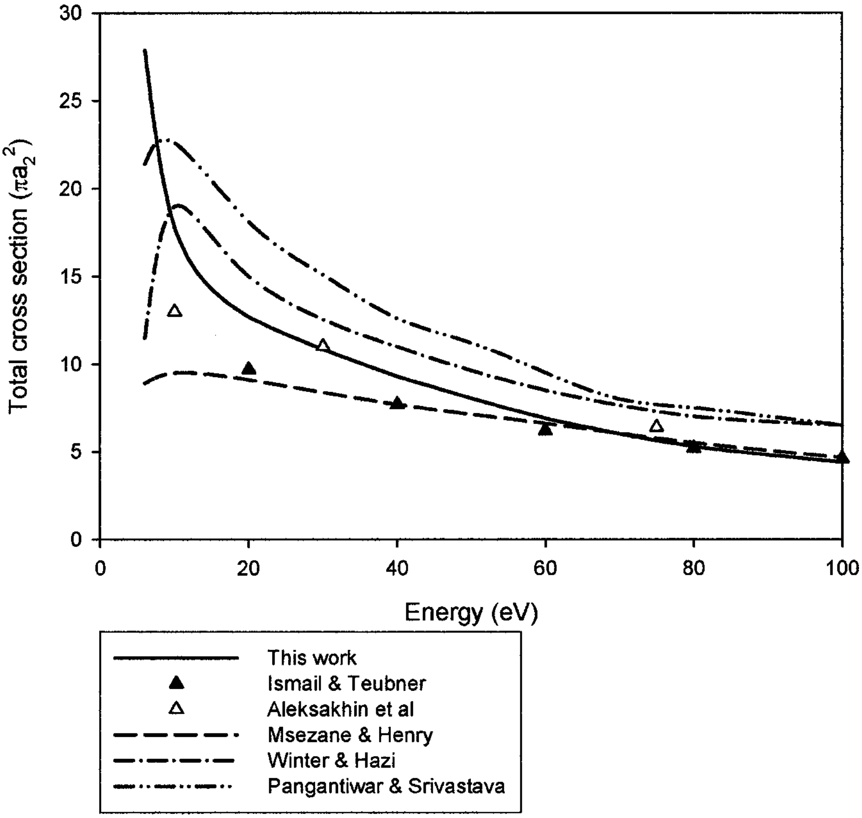

Fig. 1. Integral cross-sections for the excitation of the $3d^{10}$ 4p ^2P state. This work (–) is compared with the measurements of Ismail (▲), Aleksakhin *et al.* (△), and the calculation of Msezane and Henry (1986[a]), Winter and Hazi (– · –), Pangantiwar DWP calculation (– · · · · –).

optical oscillator strength derived from the wavefunctions used by Pangantiwar and Srivastava (1988) as is given in Ismail and Teubner (1995) work is $f_0 = 1.0$ while from Msezane and Henry (1986b) using different wavefunctions, the optical oscillator strength was 0.64. This will give lower cross-sections than those of Peterkop and Liepinsh (1979) as is shown in Fig. 1. The disagreement in the results predicted by Born approximation in the previous discussions is directly attributed to inadequacies in the wave functions used in each calculation.

3.2. Differential Cross-Sections

The present calculation for the differential cross-section of the excitation of the $3d^{10}$ 4p ^2P state in copper calculated using Eqs. (4) and (6) are given in Tables II

Table II. Differential Cross-Sections

θ (°)	6 eV	10 eV	20 eV	40 eV
0.0000	81.5156	178.7239	461.6603	1029.3945
2.0000	81.1310	175.0093	416.0410	691.3361
4.0000	79.9990	164.7417	320.9382	348.3126
6.0000	78.1823	150.0787	232.4505	190.7218
8.0000	75.7762	133.4677	167.7699	116.8177
10.0000	72.8965	116.8644	123.6169	78.0137
12.0000	69.6671	101.4681	93.5779	55.5191
14.0000	66.2092	87.8269	72.7394	41.4342
20.0000	55.4769	57.6301	38.9412	20.8339
25.0000	47.1409	41.9105	25.8422	13.5077
30.0000	39.9058	31.5324	18.3815	9.4837
40.0000	28.8977	19.5295	10.7084	5.4523
50.0000	21.5643	13.2920	7.0700	3.5775
60.0000	16.6650	9.7022	5.0732	2.5584
70.0000	13.3175	7.4701	3.8653	1.9453
80.0000	10.9691	5.9991	3.0830	1.5495
90.0000	9.2812	4.9864	2.5506	1.2808
100.0000	8.0435	4.2663	2.1750	1.0915
110.0000	7.1226	3.7422	1.9033	0.9547
120.0000	6.4316	3.3555	1.7035	0.8542
160.0000	5.0642	2.6060	1.3185	0.6607
180.0000	4.9208	2.5285	1.2788	0.6408

and III. The present data for 6 eV are shown in Fig. 2 together with those of Pangantiwar and Srivastava (1988), and the measurments of Trajmar *et al.* (1977).

The figure shows that our calculation for the differential cross-sections at 6 eV agree with the differential cross-section predicted by Pangantiwar and Srivastava

Table III. Differential Cross-Sections

θ (°)	60 eV	80 eV	100 eV
0.0000	1597.5533	2165.8187	2734.1268
2.0000	747.1041	708.3266	643.7818
6.0000	142.1737	111.0456	90.5368
10.0000	54.3591	41.3987	33.3524
14.0000	28.2719	21.3729	17.1604
30.0000	6.3559	4.7754	3.8234
50.0000	2.3897	1.7935	1.4352
70.0000	1.2983	0.9741	0.7794
90.0000	0.8545	0.6410	0.5129
110.0000	0.6368	0.4777	0.3822
130.0000	0.5202	0.3902	0.3122
150.0000	0.4580	0.3436	0.2749
180.0000	0.4273	0.3205	0.2565

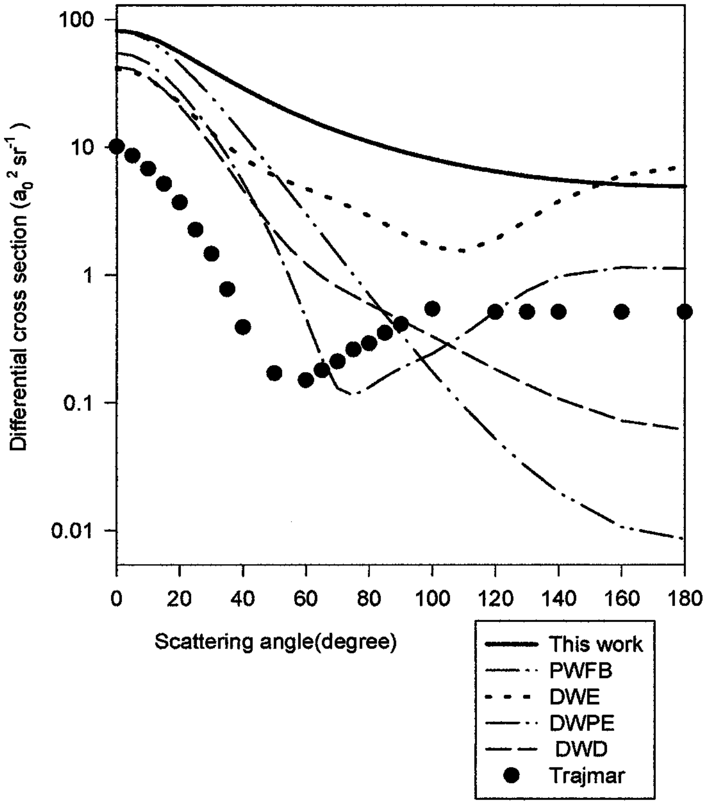

Fig. 2. Differential cross-sections at 6 eV impact energy. This work (–), the experimental results of Trajmar (•), Pangantiwar and Srivastava calculations: PWFB (– ·), DWE (· · ·), DWPE (– · ·), DWD (– –).

(1988) (PWFB) for scattering angles less than 15° and do not agree with any other results. There is clearly a large difference between the absolute values of the different results.

The present calculation at 10 eV are shown in Fig. (3). We compare our results with those of Trajmar *et al.* (1977) and of Pagantiwar and Srivastava (1988). There is good agreement between the absolute values of our calculation and the other set of calculation at scattering angles less than 18°. But the agreement with the measurments of Trajmar *et al.* (1977) is not good.

The differential cross-sections at 20 eV over the whole angular range are shown in Fig. 4(b). We compare our calculation with those of Ismail and Teubner (1995), Trajmar *et al.* (1977), Pangantiwar and Srivastava (1988). There is clearly a large diffrence between the absolute values of the two sets of measurments, the agreement of the present calculation with the measurments of Ismail and Teubner

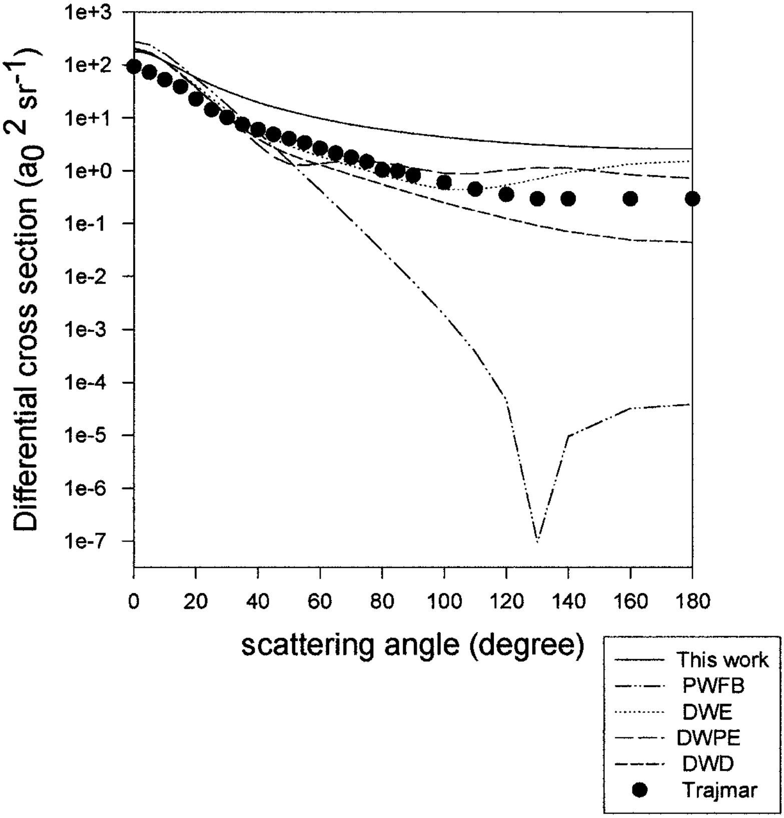

Fig. 3. Differential cross-sections at 10 eV impact energy. This work (–). The experimental results of Trajmar (•), the calculations of Pangantiwar and Srivastava calculations: PWFB (– ·· –), DWE (· · ·), DWPE (– – ·), DWD (– – –).

(1995) and with the calculation of Pangantiwar and Srivastava (1988), in particular at the forward angles (i.e.) $\theta < 15^{\circ}$ is fairly good. None of the calculations or the measurments agree at large angles.

The cross-sections at 40 eV over the whole angular range are shown in Fig. 5(a) together with the measurments of Ismail and Teubner (1995). Figure 6(a) shows the cross-section at 60 eV together with different measurments and calculation. The figure shows a good agreement between our calculation and the measurments of Ismail and Teubner (1995) again, at the forward angles, i.e. $\theta < 15^{\circ}$.

The present calculation at 80 and 100 eV are shown in Figs. 7 and 8, the figures show an agreement between our calculation and the measurments only at the forward angles, but there is no agreement with any of the other calculations for

(a)

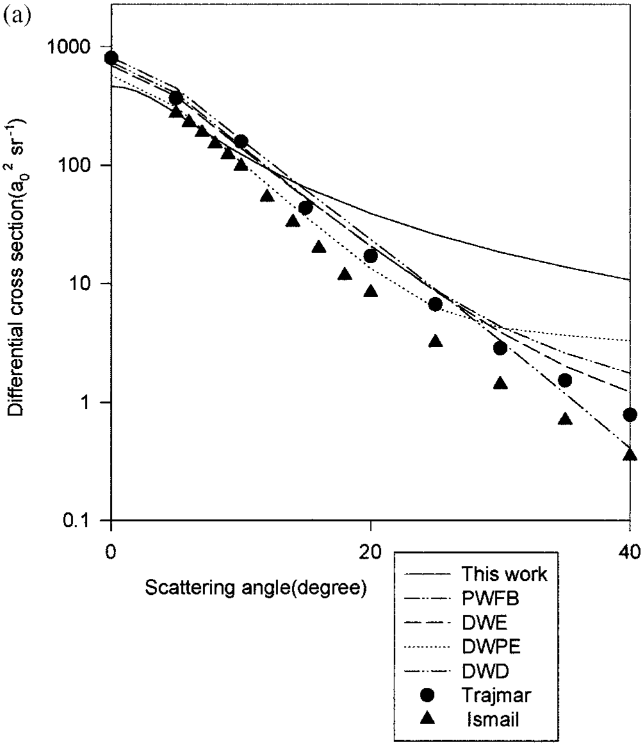

Fig. 4. (a) Differential cross-sections at 20 eV impact energy. This work (–), the experimental results of Trajmar (•), the calculations of Pangantiwar and Srivastava: PWFB (– ·· –), DWE (· · ·), DWPE (– – ·), DWD (· · ·). (b) Differential cross-sections at 20 eV impact energy.

example that of Msezane and Henry (1986b) or that of Pangantiwar and Srivastava (1988).

4. CONCLUSIONS

Born approximation predicts the calculation observations of the differential cross-sections for excitation of the 2P state at high energies and forward scattering angles. In general however, this approximation does not work for backward angle scattering due to the orthogonality of the inital and final state wavefunctions.

The success of our calculations in prediction of the total cross-section (agree with the experimental results) demonstrates the validity of the wavefunctions which we used rather than the success of a distorted wave calculation of Pangantiwar and Srivastava (1988). The agreement of our calculation for the total cross-section

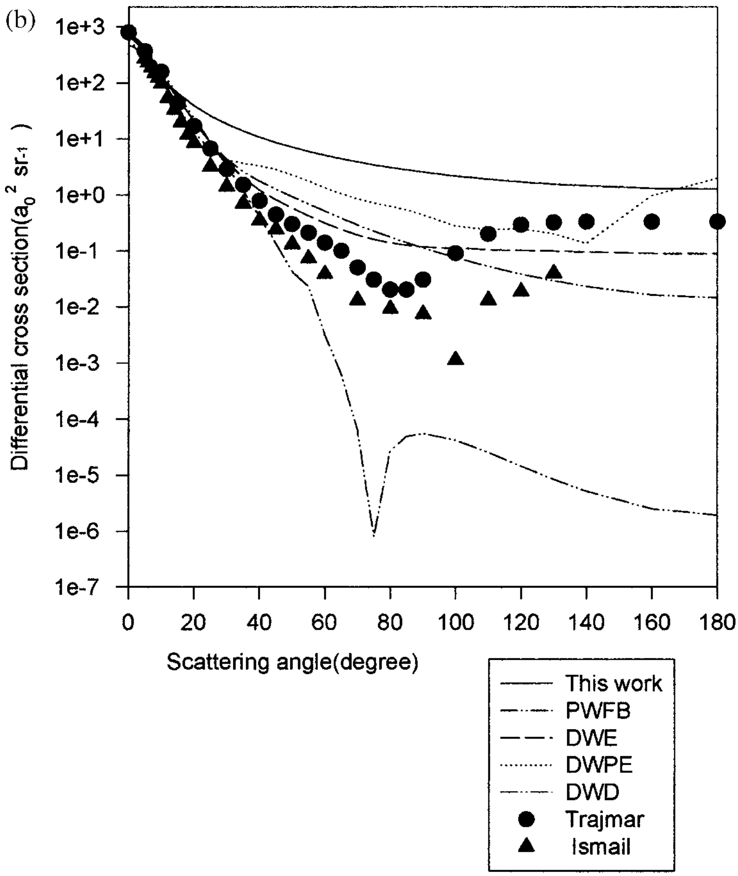

Fig. 4. (*Continued*).

with the calculation of Msezane and Henry (1986a) demonstrates the validity of the wavefunctions which they used.

The differential cross-section given by Eq. (4) measures only the magnitude of the scattering amplitudes. Born approximation can also be used to calculate the more sensitive scattering parameters derived from the electron–photon coincidence experiments. The present Born approximation calculation for the integral cross-sections for the excitation of the $3d^{10}$ 4p ^2P state at energies in excess of 20 eV give adequate results for the total cross-section. However it predicts the validity of the Born approximation calculations of the differential cross-sections for the excitation of the ^2P state at high energies and forward scattering angles.

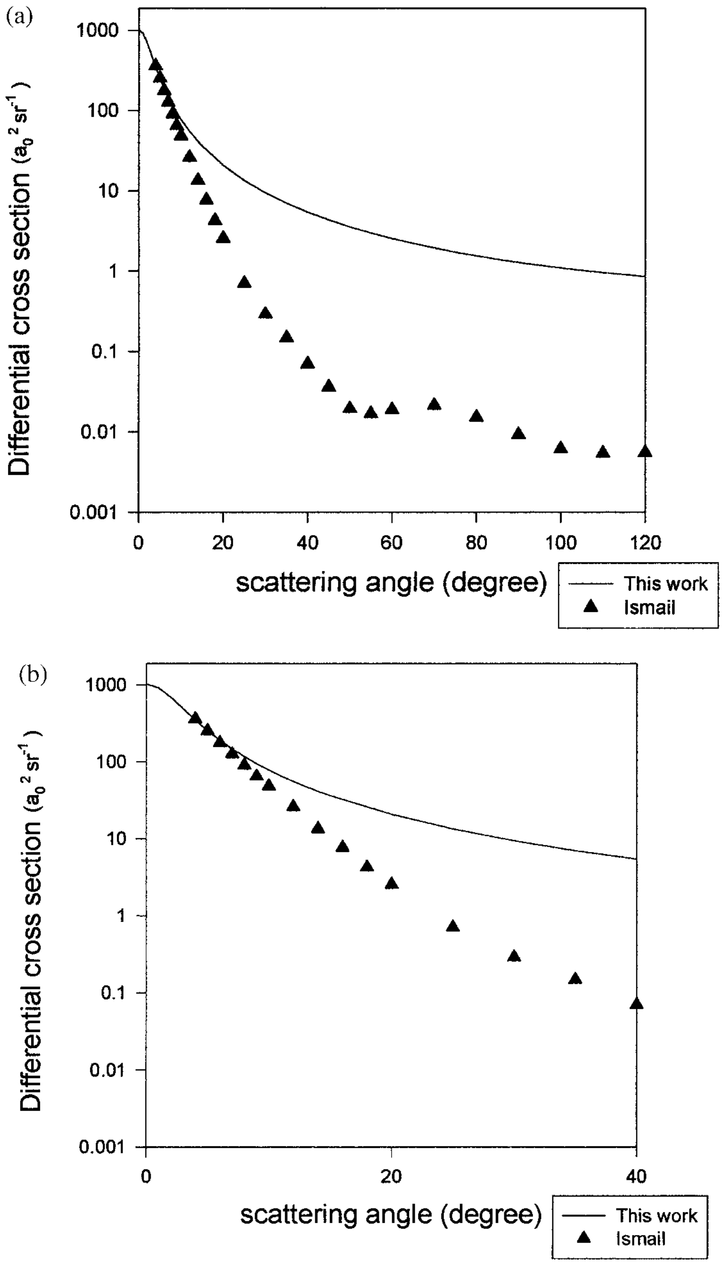

Fig. 5. (a) Differential cross-sections at 40 eV impact energy. (b) Differential cross-sections at 40 eV impact energy.

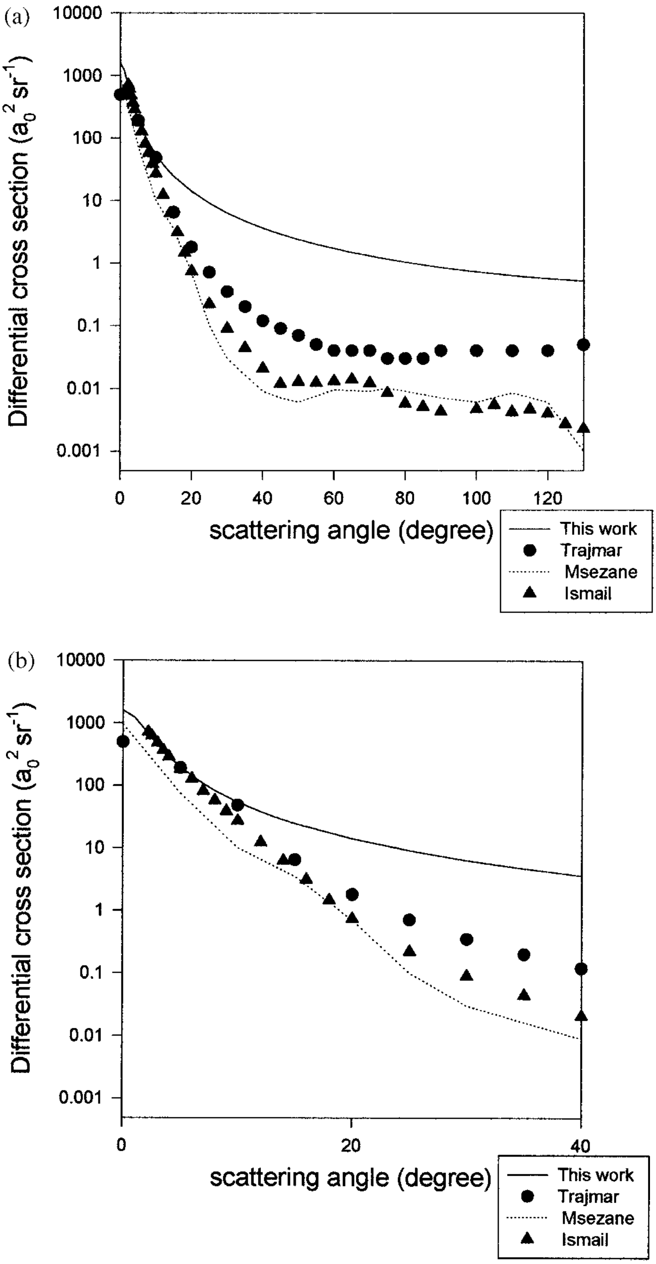

Fig. 6. (a) Differential cross-sections at 60 eV impact energy. (b) Differential cross-sections at 60 eV impact energy.

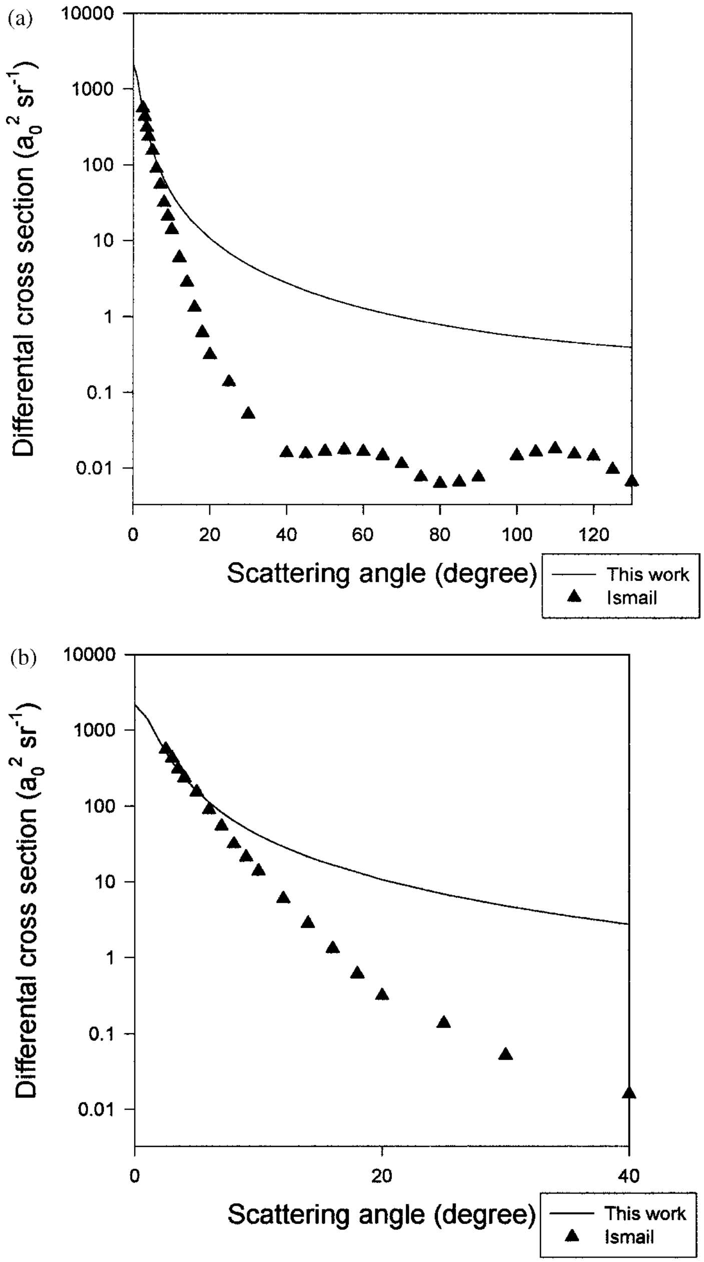

Fig. 7. (a) Differential cross-sections at 80 eV impact energy. (b) Differential cross-sections at 80 eV impact energy.

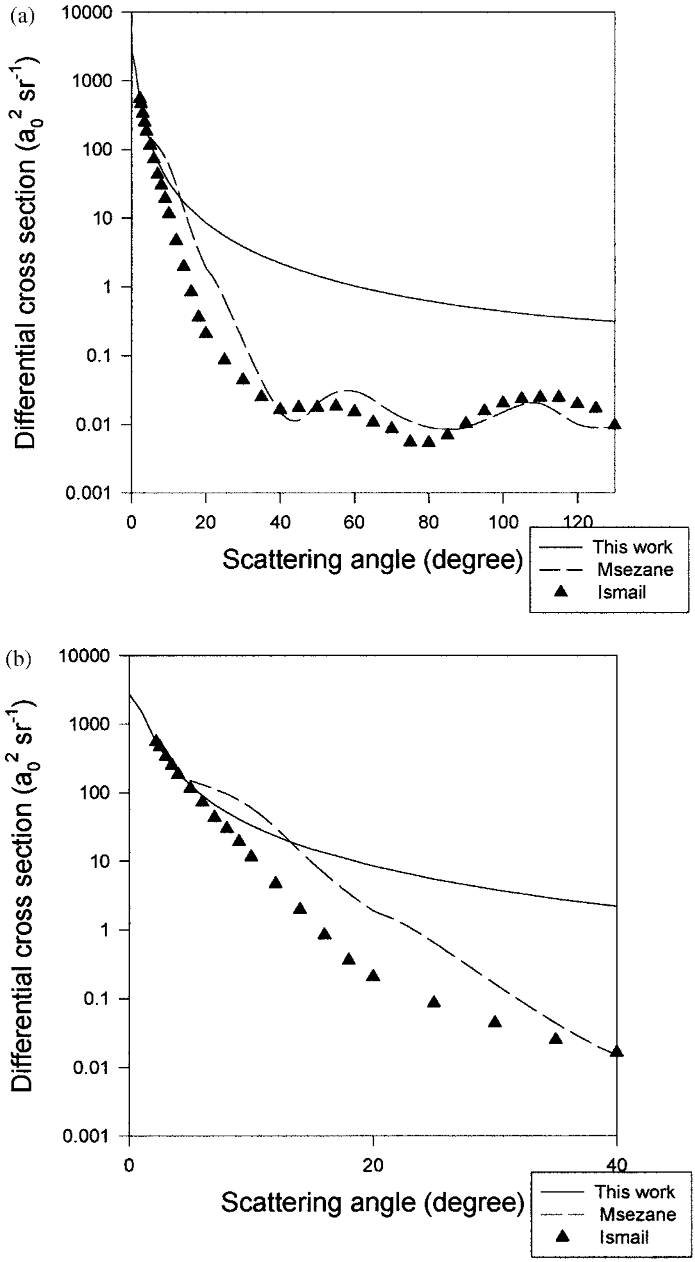

Fig. 8. (a) Differential cross-sections at 100 eV impact energy. (b) Differential cross-sections at 100 eV impact energy.

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