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Elastic scattering of electrons by argon atoms*

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Abstract. The partial wave method with a central potential has been applied to investigate the elastic scattering of electrons by the argon atoms in the intermediate energy range (100 eV—1 keV). The central potential includes the effects of the static field, exchange and polarization. The results are in good accord with recent experimental data.

Keywords. Elastic scattering; electrons; argon atoms.

1. Introduction

In the last three years a number of experimental investigations (Bromberg 1974, Gupta and Rees 1975, Dubois and Rudd 1975, Williams and Willis 1975, Jansen *et al* 1976, Vuskovic and Kurepa 1976) have been carried out to measure the absolute differential cross sections (DCS) for the elastic scattering of electrons by the argon atoms in the intermediate energy range. Prior to that only relative cross sections measured by Arnot (1931), Webb (1935) and Jost *et al* (1973) were available. At low impact energies the experimental curve of the DCS as a function of the scattering angle shows two minima. As the energy is increased, the first minimum gradually moves toward smaller angles and eventually disappears completely. Furthermore, the cross sections are sharply peaked in the forward direction. Attempts to explain the experimental curves by the first Born approximation have not been successful (Shobha 1972). This shows that, as in the case of neon atom (Jhanwar *et al* 1977), the distortion of the incident electrons wave function is important. The peaking of the DCS in the forward direction is due to the polarization and the absorption effects (Bransden and McDowell 1977).

Fink and Yates (1970) have tried to explain the observed behaviour by solving the Dirac equation in the static field approximation. However, their results are very small at low scattering angles, particularly at low impact energies. Similar results have been obtained by Walker (1971) in his relativistic calculations. Shobha (1972) applied the plane wave approximation earlier proposed by Khare and Shobha (1970), to investigate the elastic scattering of electrons by argon. This approximation which includes the polarization and exchange effects will be referred to as KSA henceforth. The results obtained in KSA (See also Khare and Shobha 1974) were compared with the available relative data of Webb (1935) and Arnot (1931). By extending the KSA we noticed that it overestimates the cross sections in most of the

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angular region. This is due to the complete neglect of the distortion of the incident electron's wave functions in KSA. The recent investigation of Lewis *et al* (1974) are based on the phenomenological optical model theory of Furness and McCarthy (1973), which contains three adjustable parameters and accounts for static field, exchange, polarization and absorption effects. Furthermore, their local exchange potential contains some errors (Riley and Truhlar 1975). Therefore, it needs a fresh investigation.

In the present paper we have employed the partial wave method to obtain DCS and the total elastic scattering cross sections in the 100 eV–1 keV energy range. To include the effect of exchange, we have followed Vanderpoorten (1975) and the non-local exchange kernel is replaced by a local exchange potential. The polarization effects have been incorporated through an energy–dependent spherically symmetric polarization potential employed by Jhanwar and Khare (1976). This potential has yielded extremly good results for the elastic scattering of electrons by the He and Ne atoms (Jhanwar and Khare 1976, Jhanwar *et al* 1977). After the completion of our work we noticed an investigation by Joachain *et al* (1977), who have followed a similar method. However, they have also included absorption effects.

2. Theory

The elastic scattering of an electron by Ar is a many-body problem. In the present investigation we have employed the optical potential approach (Mott and Massey 1965). According to this, the wave function F of the scattered electron is a solution of the following one body Schrödinger equation

$$[\nabla^2 + k^2 - V_{\text{op}}(\mathbf{r})]\, F(\mathbf{r}) = 0 \tag{1}$$

where k^2 is the energy of the incident electron and ∇^2 is the kinetic energy operator. The optical potential $V_{\text{op}}(\mathbf{r})$ is a one particle potential which is supposed to mock all the many-body effects. In general $V_{\text{op}}(\mathbf{r})$ is a complex, energy dependent and non-local potential. However, we represent $V_{\text{op}}(\mathbf{r})$ by a local energy dependent potential and employ the partial wave method to obtain $F(\mathbf{r})$. Neglecting exchange effects for the time being, replacing $V_{\text{op}}(\mathbf{r})$ by $V_{\text{op}}^{\text{D}}(\mathbf{r})$ and retaining $V_{\text{op}}(\mathbf{r})$ only up to second order we take

$$V_{\text{op}}^{D}(\mathbf{r}) = V_{\text{oo}}(\mathbf{r}) + V_{\text{dp}}(\mathbf{r}) \tag{2}$$

where $V_{\text{oo}}(\mathbf{r})$ is the static potential given by $\langle 0 \mid V(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N; \mathbf{r}_{N+1}) \mid 0 \rangle$. Here $|0\rangle$ is the ground state wave function of the target atom having N electrons (for argon N=18) and $V(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N; \mathbf{r}_{N+1})$ is the interaction potential between the target and the incident electron. We have represented $V_{\text{dp}}(\mathbf{r})$ by a real spherically symmetric potential given by (Jhanwar and Khare 1976).

$$V_{\text{dp}}(r) = -\frac{\alpha_d r^2}{(r^2 + d^2)^3} - \frac{\alpha_q r^4}{(r^2 + d^2)^5} \tag{3}$$

with $d = 0{\cdot}75\ \text{k}/\Delta$

where α_d and α_q are, respectively, the dipole and quadrupole polarizabilities of the atom. $\triangle$ represents the mean excitation energy of the atom and is equal to exp $[L(-1)/S(-1)]$. Here $L(-1)$ and $S(-1)$ are properties of the atom and require oscillator strength distribution for their determination (Inokuti *et al* 1967).

Let us now consider exchange effects. In principle the exchange potential is a non-local potential and its application at intermediate energies is time consuming. Therefore in the present investigation we have followed Vanderpoorten (1975) and constructed a local exchange potential given as

$$V_{ex}(r) = \tfrac{1}{2}\,[k^2 - V_{op}^D - \{(k^2 - V_{op}^D)^2 + 32\pi\,\rho(\mathbf{r})\}^{\frac{1}{2}}] \tag{4}$$

where ρ (**r**) is the spherically symmetric charge distribution of the target atom. Thus we have replaced the target atom by a real spherically symmetric potential $V_{op}(\mathbf{r})$ which is a sum of V_{op}^D and exchange potential. Now, the use of the partial wave method reduces (1) to a one-dimensional radial equation given by

$$\left[\frac{d^2}{dr^2} + k^2 - V_{op}(r) - \frac{l(l+1)}{r^2}\right] f_l(r) = 0 \tag{5}$$

where $f_l(r)$ has the asymptotic form

$$f_l(r) \underset{r\to\infty}{\sim} 1/k \sin(kr - l\pi/2 + \eta_l). \tag{6}$$

η_l is the lth order phase shift and is due to the presence of the potential $V_{op}(r)$ in eq. (5).

3. Calculation

We have applied the model presented in section 2 to study the elastic scattering of electrons by argon atoms. In order to calculate $V_{oo}(r)$ and $V_{ex}(r)$ we have employed the wave function as given by Sheorey (1969). The wave function may be written as

$$\psi_{Ar}(\mathbf{r}_1, \ldots, \mathbf{r}_{18}) = \phi_{1s}(\mathbf{r}_1)\,\phi_{1s}(\mathbf{r}_2) \ldots \phi_{3p}(\mathbf{r}_{18}) \tag{7}$$

where

$$\phi_{nl}(\mathbf{r}) = R_{nl}(r)\; Y_{lm}(\hat{r})$$

$Y_{lm}(\hat{r})$ are the normalized spherical harmonics and the radial functions $R_{nl}(r)$ are linear combinations of the functions of the type

$$R_{nl}(r) = N_{nl}\, r^{n-1} \exp(-\alpha_{nl}\, r) \tag{8}$$

N_{nl} are the normalization constants and are given by

$$N_{nl} = \left[\frac{(2\alpha_{nl})^{2n+1}}{(2n)!}\right]^{\frac{1}{2}}. \tag{9}$$

Since for a many-electron atom, hydrogenic radial functions (8) do not form an orthogonal basis set, the basic functions are, therefore, orthogonalized by applying the Schmidt orthogonalization procedure to orbitals with the same angular momentum l, starting with those of lowest principal quantum number n. Thus the various normalized radial orbitals are given by

$$R_{2s}(r)=C_{2s-2s}R_{2s}(r)+C_{2s-1s}R_{1s}(r) \tag{10}$$

$$R_{3s}(r)=C_{3s-3s}R_{3s}(r)+C_{3s-2s}R_{2s}(r)+C_{3s-1s}R_{1s}(r) \tag{11}$$

$$R_{3p}(r)=C_{3p-3p}R_{3p}(r)+C_{3p-2p}R_{2p}(r) \tag{12}$$

where $C_{nl-n'l}$ are the orthogonality coefficients. The optimum values of the orbital exponents α_{nl} are determined by minimizing the total energy of the system. The values of α_{nl} and $C_{nl-n'l}$ are given by Sheorey (1969).

To obtain the $V_{\mathrm{dp}}(r)$ we have taken $\alpha_d=11{\cdot}0$ and $\alpha_q=46{\cdot}501$ (Khare and Shobha 1974). To calculate $\triangle$ we have used the values of $L(-1)$ and $S(-1)$ given by Dehmer and Saxon (1973) and obtained $\triangle=1{\cdot}624$ Rydbergs. Using the form of $V_{\mathrm{op}}(r)$ thus obtained, eq. (5) is solved numerically for the first M values of l and the phase shifts η_l are determined. In order to illustrate the importance of polarization effects, the phase shifts are also obtained by taking the static potential only in $V_{\mathrm{op}}(r)$. The scattering amplitude is obtained from the expression

$$f(\theta)=\frac{1}{k}\sum_{l=0}^{M}(2l+1)e^{i\eta_l}\sin\eta_l P_l(\cos\theta)+f_{dp}^{B}(\theta)$$

$$-\frac{1}{k}\sum_{l=0}^{M}(2l+1)\eta_l{}^{B}P_l(\cos\theta) \tag{13}$$

where $f_{\mathrm{dp}}^{B}(\theta)$ represents the scattering amplitude in the Born approximation due to potential $V_{\mathrm{dp}}(r)$ and $\eta_l{}^{B}$ are the corresponding Born phase shifts. M is the smallest integer such that the phase shift η_M is equal to the Born phase shift η_M^B (within 5%). The value of M is energy-dependent and increases with the energy. Its values at energies ranging from 100 eV to 1 keV are listed in table 1. It may be mentioned that the values of $\eta_l{}^{B}$ for $l=0$ to M are small. Hence in the third term of eq. (13), $e^{i\eta_l^B}\sin\eta_l{}^{B}$ has been replaced by $\eta_l{}^{B}$. The Born phase shifts are obtained by the relation

$$\eta_l{}^{B}=-k\int_0^{\infty}r^2V_{\mathrm{dp}}(r)\,[j_l(kr)]^2\,dr \tag{14}$$

Table 1. The value of the integer M for which the phase shift η_M, obtained by numerical solution of eq. (5) is equal to the Born phase shift η_M^B (within 5%) for various impact energies.

E(eV)	100	150	200	300	400	500	800	1000
M	11	12	15	16	18	20	28	29

where $j_l(kr)$ are the spherical Bessel functions. By substituting the expression (3) for $V_{dp}(r)$ in the relation (13), we have obtained an analytical expression for the η_l^B. The details of the evaluation of the integral is given elsewhere for the case of neon atoms (Jhanwar *et al* 1977). The DCS, $I(\theta)$, are obtained by taking the modulus square of the scattering amplitude $f(\theta)$. Finally, the total elastic cross section, $Q_{el}(E)$, is obtained with the help of the optical theorem

$$Q_{el}(E)=\frac{4\pi}{k} I_m f(\theta=0) \tag{15}$$

where $I_m f(\theta=0)$ represents the imaginary part of the forward elastic scattering amplitude.

4. Results and discussions

In figures 1-8 we have shown our present results of DCS obtained with only the static field $V_{oo}(r)$ and with the complete potential $V_{op}(r)$ by the curves *A* and *B*, respectively.

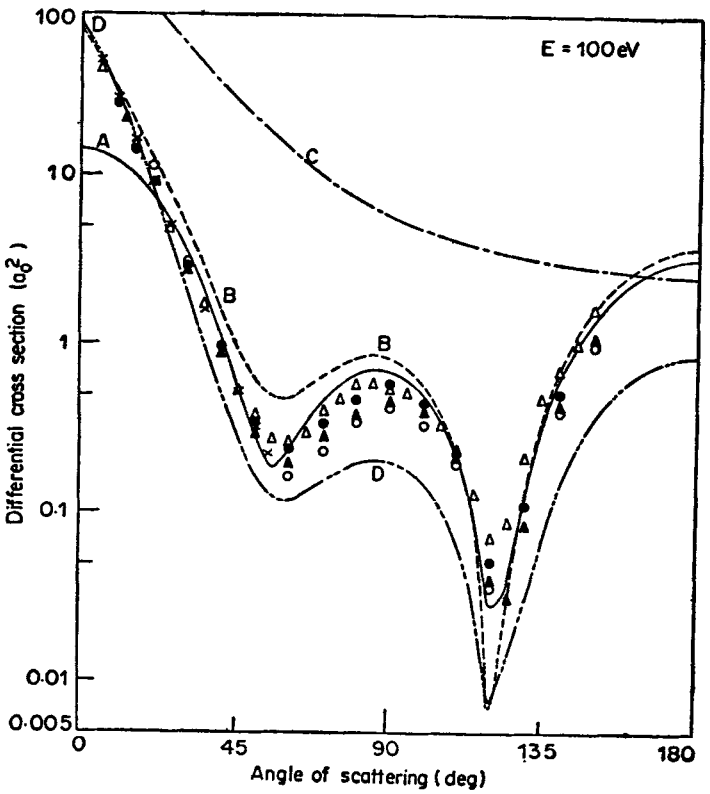

Figure 1. Differential cross sections for electrons elastically scattered by argon atoms at $E=100$ eV. *Theory:* *A*—Present results in static field approximation; *B*—Present results in static field+polarization+exchange approximation; *C*—Khare and Shobha (1974); *D*—Joachain *et al* (1977). *Exp. data:* ● Gupta and Rees 1975 (experimental accuracy ±10%); ▲ Dubois and Rudd 1975 (experimental accuracy ±12%); o—Williams and Willis 1975 (experimental accuracy ±8%); △—Vuskovic and Kurepa 1976 (experimental accuracy ±17·5%); x—Jansen *et al* 1976 (experimental accuracy ±6·5%).

For comparison, we have also included in the figures the KSA results and the recently obtained results of Joachain *et al* (1977). It is evident from the figures that KSA fails completely in explaining the experimental results. On the other hand the partial wave method, even with the static field alone (curves A), considerably improves the agreement between theory and experiment. All the minima and maxima are very well reproduced. However, as expected curves A lie below the experimental data at low angles ($<20°$). The inclusion of polarization and exchange effects (curves B) yields good agreement between theory and experiment at low angles. However at θ equal to 5°, the experimental points lie above the curves B. With the increase of incident energy the difference between the curves A and B decreases. The main difference being at low angles where the curves B yield much better agreement with the experimental data. This shows the importance of the polarization effects particularly at low angles. Let us now consider the results of Joachain *et al* (1977) shown by the curves D. From the figures it is clear that the curves D lie, in general, below the curves B and most of the experimental data lie between the curves B and D. However with the increase of the impact energy the difference between the two curves decreases and both of them yield good agreement with the recent experimental data. In table 2 we have compared the present values of the total elastic cross sections with the experimental data (Jansen 1975, Dubois and Rudd 1975) and theoretical value

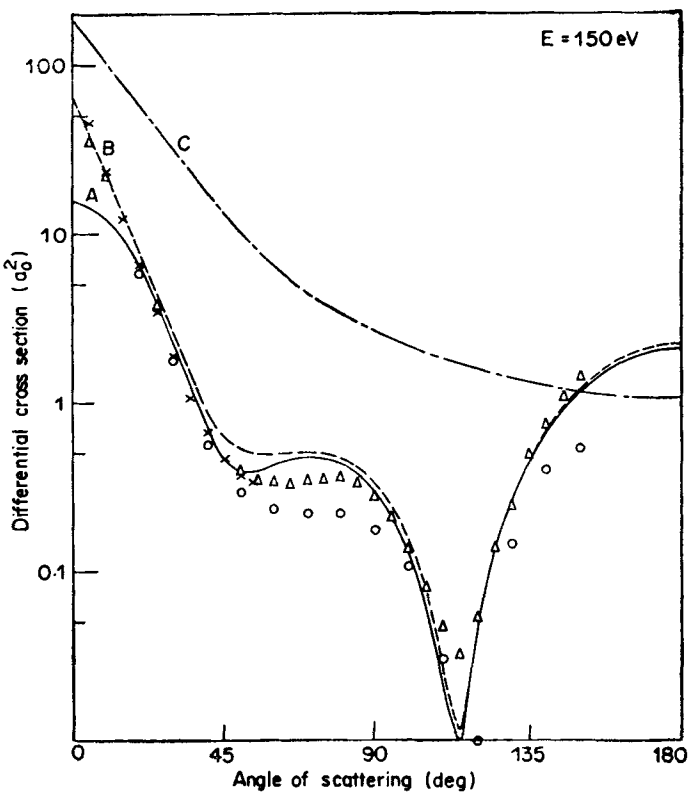

Figure 2. Differential cross sections for electrons elastically scattered by argon atoms at $E=150$ eV. *Theory: A, B, C* and *D*—Same as in figure 1. *Exp. data:* o, △ and x—same as in figure 1.

(Joachain *et al* 1977). We have also obtained the total cross section Q_{el} by integrating the DCS. These values do not differ by more than 0·5% from the values shown in the second column of table 2. From the table one can notice that the present values, except at 100 eV, are in good agreement with the experimental data. Finally we infer that the present method yields good agreement between the theory and

Table 2. Total elastic cross sections (in units of a_0^2) for electron-argon scattering.

	Theoretical values		Experimental values	
E (eV)	Present results	Joachain *et al* (1977)	Jansen (1975)	Dubois and Rudd (1975)
100	22·97	13·7	13·6	15·2
150	15·63	—	12·0	—
200	12·34	9·96	10·8	10·3
300	9·35	8·35	9·14	—
400	7·87	7·35	8·01	—
500	6·91	6·63	7·12	7·25
800	5·26	5·23	—	5·13
1000	4·60	4·62	4·68	—

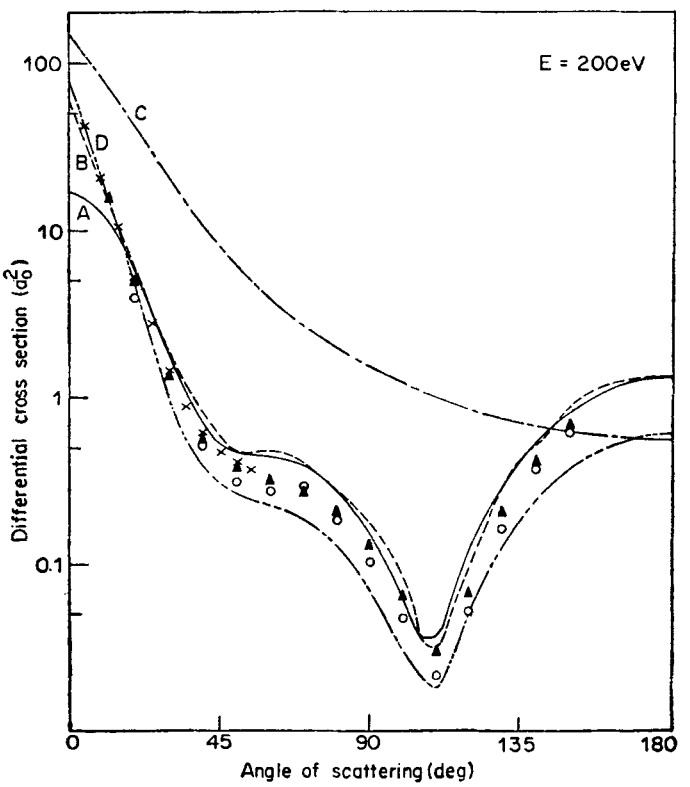

Figure 3. Differential cross section for electrons elastically scattered by argon atoms at E=200 eV. *Theory:* *A*, *B*, *C* and *D*—same as in figure 1. *Exp. data:* ▲, o and x—same as in figure 1.

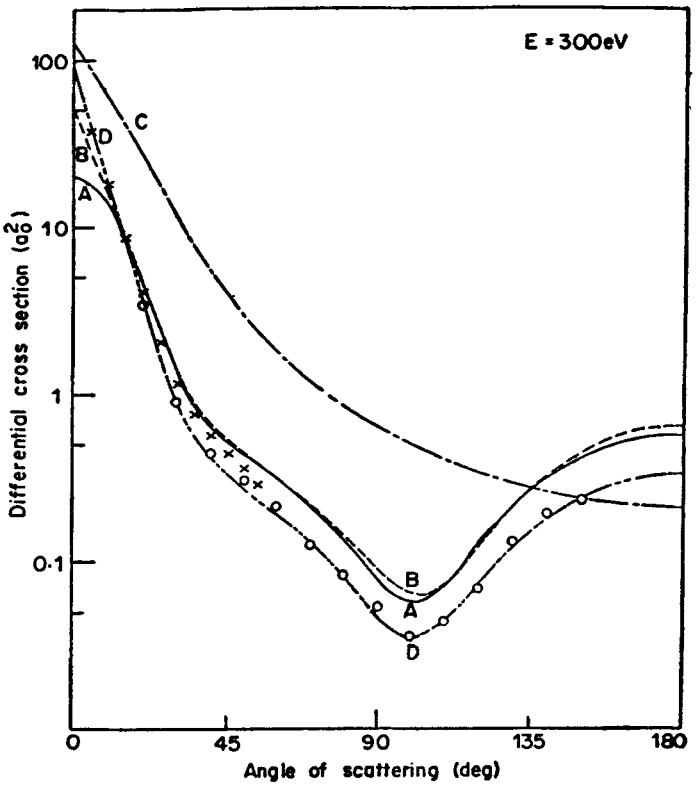

Figure 4. Differential cross sections for electrons elastically scattered by argon atoms at $E=300$ eV. *Theory: A, B, C* and *D*—same as in figure 1. *Exp. data:* o and x—same as in figure 1.

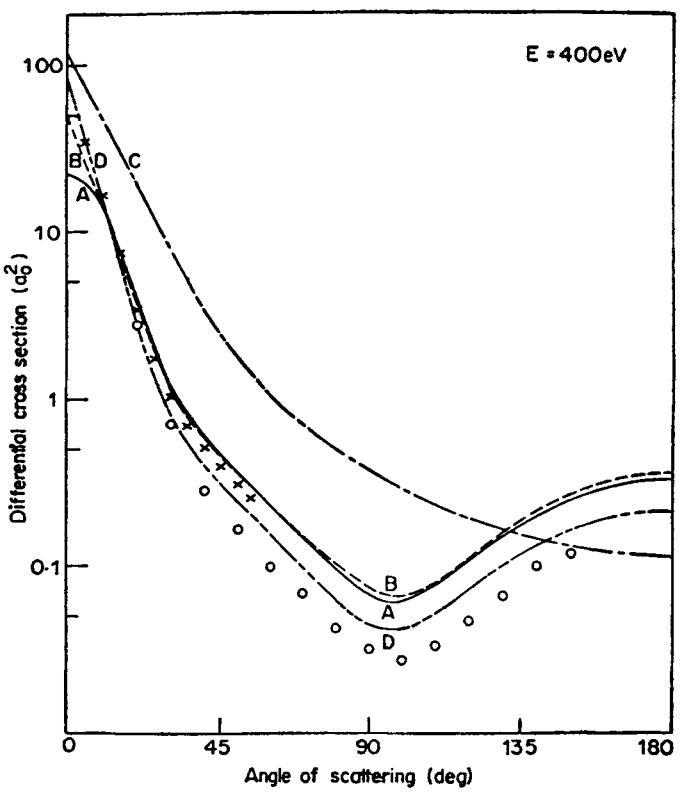

Figure 5. Differential cross sections for electrons elastically scattered by argon atoms at $E=400$ eV. *Theory: A, B, C* and *D*—same as in figure 1. *Exp. data:* o and x—same as in figure 1.

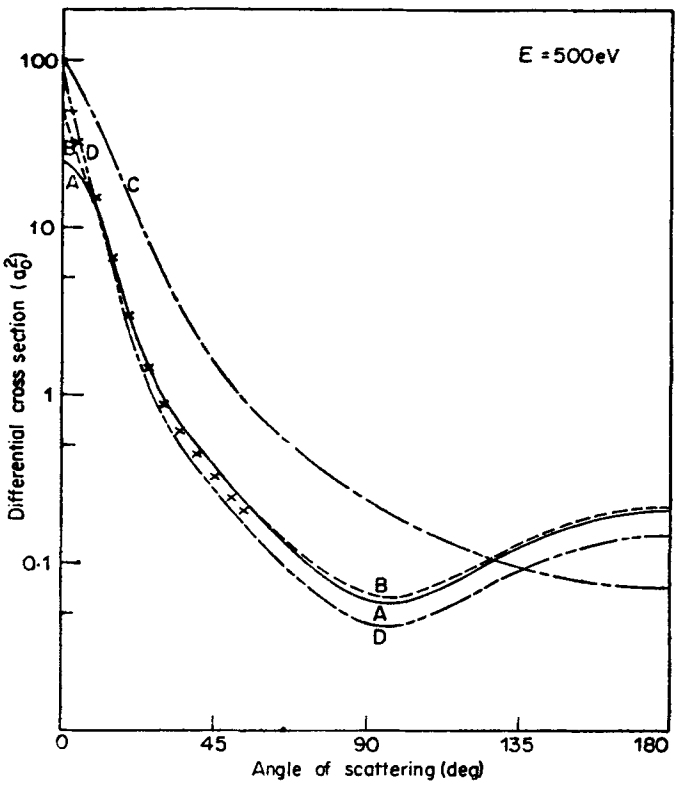

Figure 6. Differential cross sections for electrons elastically scattered by argon atoms at $E = 500$ eV. *Theory:* *A*, *B*, *C* and *D*— same as in figure 1. *Exp. data:* x same as in figure 1.

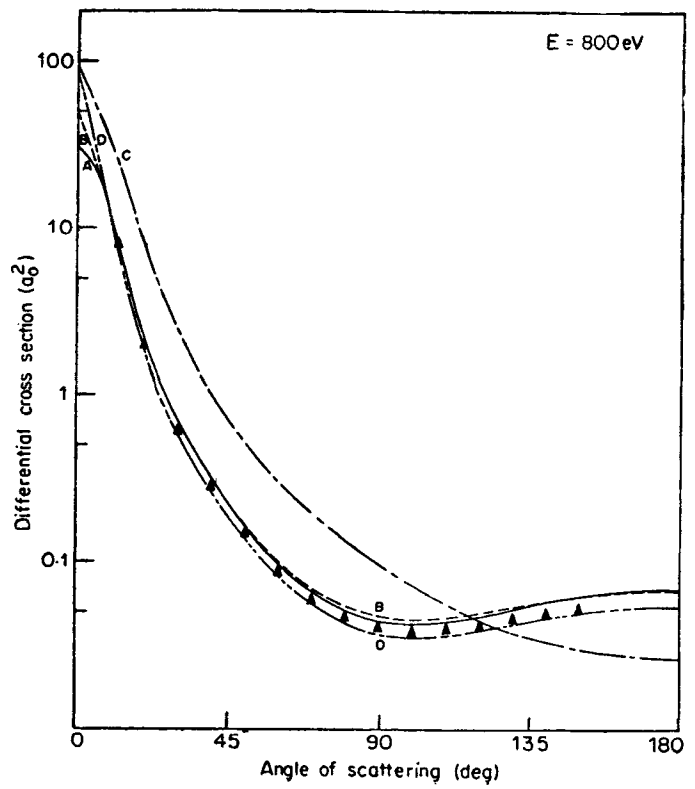

Figure 7. Differential cross sections for electrons elastically scattered by argon atoms at $E = 800$ eV. *Theory:* *A*, *B*, *C* and *D*— same as in figure 1. *Exp. data:* ▲ — same as in figure 1.

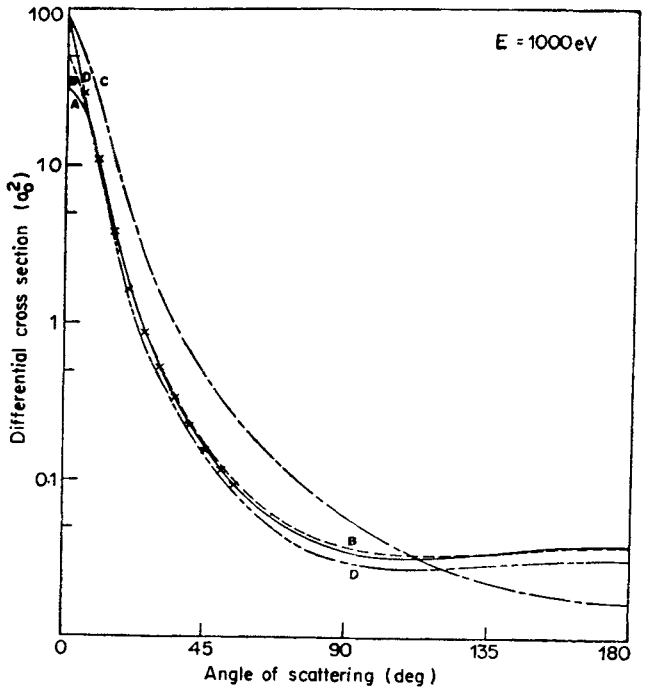

Figure 8. Differential cross section for electrons elastically scattered by argon atoms at E=1 keV. *Theory: A, B, C* and *D*—same as in figure 1. *Exp. data:* x—same as in figure 1.

recent experiments for DCS as well as total elastic cross sections for the elastic scattering of electrons on the argon atoms for energies greater than 100 eV. Work is in progress to extend the above method for the elastic scattering of electrons by heavier noble gases, namely, krypton and xenon.

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