Spin polarization for electrons scattering from argon atom

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Spin polarization parameter for the scattering of electrons from argon atom in the energy range of 3-300eV are calculated using the relativistic Dirac equation.The interest of spin polarization calculation is to obtain a complete information about the projectile-target interaction and scattering process .The projectile-target interaction is represented by a total potential which is consist of a sum of model potentials. The spin polarization parameter S for electrons scattering is found to be in good agreement with the other calculated values.

استقطاب البرم للالكترونات المستطاره من ذرة الاركون

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الخلاصة

لقد تم حساب معامل استقطاب البرم لاستطارة الالكترونات من ذرة الاركون في مدى طـاقي مـن 3-300 الكترون فولت باستخدام معادلة ديراك النسبية.ان اهمية حساب استقطاب البرم هو للحصول على المعلومـه الكامله حول تفاعل الجسيم المقذوف مع الهدف وحول عملية الاستطاره .ان تفاعل الجسـيم المقـذوف مـع الهدف مثل بجهد متكون من مجموعة نماذج جهدية.ان القيم المحسوبه لمعامل اسـتقطاب البـرم لاسـتطارة الالكترونات وجدت في حالة اتفاق جيد مع النتائج المحسوبه الاخرى.

1.INTRODUCTION:

Scattering of electrons by argon atom has been an intensively studied problem for a long time because there is a lot of calculations have been made for this atom also argon may play an exceptional role in exhibiting the Ramsauer-Townsend minimum for the scattering of both the electrons and the positrons [1].In the present work,the investigation performed on the same scattering problem using the relativistic approach, by solving the Dirac equation, which provides, in its standard formulation, the interaction effects of the projectile's spin.During the scattering of electrons their magnetic moments interact with the magnetic field generated by the orbital motion of these particles with respect to the target atom, leading to the well-known spin-orbit interaction term. Hence, even though the incident beam of projectiles may be unpolarized, the spin-orbit interaction can adjust the spins of the scattered particles in a preferred direction causing a net spin polarization.The study of spin polarization of the incident projectiles according to scattering provides more detailed information about the projectile-target interaction and scattering process.The spin polarization of electrons during scattering by a central field was first investigated by Mott [2],using a relativistic treatment based on the theory of Dirac[3].In the present work,the calculations start with the Dirac equation to describe the scattering system and calculate the sherman function S according to scattering in the impact energy range of 3-300 eV.

Sec.2, explain the theory used in this work,where the computational method ,the calculated spin polarization parameter and the interaction between an electron and a target atom describe.While sec.3, deals with the results and discussion obtained from the calculated results , the conclusions are given in sec.4 .

2. THEORY

The Dirac equation for a central potential can be set of two equations [4]:

$$(g_l^{\pm})^{//} + [K^2 - l(l+1)/r^2 - U_l^{\pm}(r)]g_l^{\pm}(r) = 0 \quad \text{--------(1)}$$

Where $g_l^{\pm}$ is related to the radial part $G_l^{\pm}$ of the large component of wave function as introduced by Sultana et.al.[4].The functions $U_l^{\pm}$ are the effective Dirac potentials and are given by P.Kumar et.al.[5].The proper solution of Eq.(1) behaves asymptotically as [4]:

$$g_l^{\pm}(K,r) = Kr[j_l(Kr) - \tan(\delta_l^{\pm})\eta_l(Kr)] \text{ , when } r \to \infty \quad \text{-----------(2)}$$

Where j_l and η_l are the spherical Bessel functions of the first and second kind,respectively.The plus and the minus signs attached to the phase shifts $\delta_l^{\pm}$ correspond to incident particles with spin up and with spin down,respectively.The phase shifts $\delta_l^{\pm}$ can be obtained from the values of the radial wave function $g_l^{\pm}$ at the two adjacent points r and r+h (h « r) at very large r as [4] :

$$\tan\delta_l^{\pm} = -\frac{(r+h)g_l^{\pm}(r)j_l[K(r+h)] - rg_l^{\pm}(r+h)j_l(Kr)}{rg_l^{\pm}(r+h)\eta_l(Kr) - (r+h)g_l^{\pm}(r)\eta_l[K(r+h)]} \quad \text{--------------(3)}$$

In the present calculation,the wave functions $g_l^{\pm}$ are obtained by numerical integration of Eq.(1) using Numerov's method[4].The two complex scattering amplitudes $f(K,\theta)$ (the direct amplitude) and $g(K,\theta)$ (the spin-flip amplitude) are defined as[6]:

$$f(K,\theta) = \frac{1}{2iK}\sum_{l=0}^{\infty}\{(l+1)[\exp(2i\delta_l^{+}) - 1] + l[\exp(2i\delta_l^{-} - 1)]\}P_l(\cos\theta) \quad \text{-------(4)}$$

And

$$g(K,\theta) = \frac{1}{2iK}\sum_{l=1}^{\infty}[\exp(2i\delta_l^{-}) - \exp(2i\delta_l^{+})]p_l^1(\cos\theta) \quad \text{------------(5)}$$

Where θ is the scattering angle and $P_l(\cos\theta)$ and $p_l^1(\cos\theta)$ are the Legendre polynomial and the Legendre associated functions,respectively.The elastic differential cross section for scattering of the unpolarized incident electron beam is given by[4]:

$$\sigma_u(\theta) = \frac{d\sigma}{d\Omega} = |f|^2 + |g|^2 \quad \text{--------------------(6)}$$

And the spin polarization parameter $S(\theta)$ (Sherman function) had the form [7]:

$$S(\theta) = \frac{i(fg^* - f^*g)}{\sigma_u(\theta)} \quad \text{-------------(7)}$$

The Sherman function $S(\theta)$ describes the spin polarization parameter of the scattered electrons if the incident electron beam is unpolarized .The interaction between an electron and a target atom is describe by an effective potential $V(r)$ which is chosen to be a sum of three terms, the static $V_{st}(r)$,exchange $V_{ex}(r)$,and polarization $V_{cpol}(r)$ potentials .These effective potential terms are functions of the electronic density of the target and approximately account for the dynamics of the collision. The electrostatic interaction energy between the projectile and the target atom obtained by [8]:

$$V_{st}(r) = Z_o e\varphi(r) = Z_o e[\varphi_n(r) + \varphi_e(r)] \quad \text{-----------------(8)}$$

Where $Z_o e$ is the charge of the projectile and $\varphi(r)$ is the electrostatic potential of the target atom which is express as the sum of contributions from the nucleus and the electron cloud, $\varphi_n(r)$ and $\varphi_e(r)$, respectively , by [8]:

$$\varphi_n(r) = e\left(\frac{1}{r}\int_0^r \rho_n(r^/)4\pi r^{/2}dr^/ + \int_r^\infty \rho_n(r^/)4\pi r^/ dr^/\right) \quad \text{--------------(9)}$$

And

$$\varphi_e(r) = -e\left(\frac{1}{r}\int_0^r \rho_e(r^/)4\pi r^{/2}dr^/ + \int_r^\infty \rho_e(r^/)4\pi r^/ dr^/\right) \quad \text{--------------(10)}$$

Where $\rho_n(r)$ and $\rho_e(r)$ denote the space densities (particles per unit volume) of protons in the nucleus and orbital electrons, respectively.To quantify the screening of the nuclear charge by the atomic electrons, there is a screening function, $\chi(r)$, defined as the fraction of the nuclear charge seen by a particle at a distance *r* from the center of the nucleus,and obtained by [8]:

$$\chi(r) = \frac{r}{Ze}\varphi(r) \quad \text{---------------------(11)}$$

The electrostatic potential and the particle densities of the atom are linked by Poisson's equation which for spherically symmetric systems and $(r \succ 0)$ simplifies to:

$$\rho_n(r) - \rho_e(r) = -\frac{1}{4\pi er}\frac{d^2}{dr^2}[r\varphi(r)] = -\frac{Z}{4\pi r}\frac{d^2\chi(r)}{dr^2} \quad \text{---------------(12)}$$

Where $\rho_n(r)$ obtained by Fermi distribution as :

$$\rho_n(r) = \frac{\rho_o}{\exp[(r - R_n)/\mathrm{Z}] + 1} \quad \text{------------------------(13)}$$

Where $Z = t/(4\ln 3) = 0.546\times10^{-13}cm$ and $t = 2.4\times10^{-13}cm$ (the skin thickness) defined as the distance over which the density drops from 0.9 to 0.1 of its central value, also $R_n = 1.07\times10^{-13}A^{1/3}cm$, is the mean radius (half-density radius). The constant ρ_o, which is twice the proton density at $r = R_n$, is to be determined by normalization. The electrostatic potential of the Fermi distribution, $\varphi_n(r)$,has to be calculated numerically.For $\rho_e(r)$ in the present work,where have been used the most accurate electron densities available for free atoms which obtained from self-consistent relativistic Dirac–Fock (DF) calculations [9].The same density $\rho_e(r)$ are used to obtain the electron exchange and correlation potential .The exchange potential model of Furness and McCarthy [10] which is local approximation to the exchange interaction are used to performing the calculations and given by:

$$V_{ex}(r)=\frac{1}{2}[E-V_{st}(r)]-\frac{1}{2}\{[E-V_{st}(r)]^2+4\pi a_o e^4\rho_e(r)\}^{\frac{1}{2}} \quad \text{-----------(14)}$$

Where E is the total energy of the projectile .For the polarization potential $V_{cpol}(r)$,a parameter-free polarization potential based on the correlation energy of the target atom are used.It has two components, the short-range $V_{SR}(r)$ and the long-range $V_{LR}(r)$ parts and given by [5] :

$$V_{cpol}(r)=\begin{Bmatrix} V_{cor.}^{SR}(r) & ,r<r_c \\ V_{pol}^{LR}(r) & ,r\geq r_c \end{Bmatrix} \quad \text{-------------------------(15)}$$

Here, r_c is the point where the two forms cross each other for the first time. The short-range form for electron scattering from atoms is based on the free electron gas exchange energy functions of R.Baer and D.Neuhauser [11] mixed with the free electron gas exchange energy functions of R.Armiento and A.E.Mattsson [12] and given by:

$$V_{cor.}^{SR}(r)=\left[\frac{d}{d_o+d_1 r_s+r_s^2}\right]\cdot\left[\frac{c_3}{\sqrt{c_5}}\right]-$$

$$\frac{r_s}{3}\left[\left\{\frac{d}{d_o+d_1 r_s+r_s^2}\right\}\cdot\left\{\frac{c_1\cdot c_2-c_3\cdot c_4}{c_5}\right\}-\left\{\frac{d(d_o+2r_s)}{(d_o+d_1 r_s+r_s^2)^2}\right\}\cdot\left\{\frac{c_3}{\sqrt{c_5}}\right\}\right] \quad \text{-------(16)}$$

Where $d=3.4602, d_o=3.2$ and $d_1=-0.9$ and c_1-c_5 represented by the equations:

$$c_1=r_s^2+e_4 r_s^{3/2}+e_5 r_s+e_6\sqrt{r_s} \quad \text{----------------(17)}$$

$$c_2=e_1+\frac{e_2}{2\sqrt{r_s}} \quad \text{----------------(18)}$$

$$c_3=e_1 r_s+e_2\sqrt{r_s}+e_3 \quad \text{----------------(19)}$$

$$c_4=2r_s+\frac{3e_4\sqrt{r_s}}{2}+e_5+\frac{e_6}{2\sqrt{r_s}} \quad \text{----------------(20)}$$

$$c_5=\left(r_s^2+e_4 r_s^{3/2}+e_5 r_s+e_6\sqrt{r_s}\right)^2 \quad \text{----------------(21)}$$

With:

$e_1=-1.81942, e_2=2.74122, e_3=-14.4288, e_4=0.537230, e_5=1.28184 \, and \, e_6=20.4048$.

Where $r_S=\{3/[4\pi\rho_e(\mathrm{r})]\}^{1/3}$, $\rho_e(r)$ is the undistorted electronic density of the target.The long-range form of polarization potential is given by Buckingham model[8]:

$$V_{pol}^{LR}(r)=\frac{-\alpha_d e^4}{2(r^2+d^2)^2} \quad \text{----------------------(22)}$$

Where (α_d) is the dipole polarizability and (d) is the cutoff radius.For present calculations,the value of (α_d) is taken as (10.77 a.u.)[13].And the value of (d) is taken as (7.76 a.u.) [13].

3. RESULTS AND DISCUSSION

In the present work the values of the spin polarization $S(\theta)$ for elastic scattering of electrons from argon at various impact energies between (3-300eV) are calculated relativistically by using the interaction potential in the Dirac equation where the results are compared with a theoretical values of Nahar and Wadehra [4] ,these results are shown in figure1(a-l).Where the calculated values of spin polarization parameter agree reasonably well with the available theoritical values of Nahar and Wadehra [4] except at low impact energies ($\leq$ 5 eV) in small and large angles , these difference between my results and the results of Nahar and Wadehra [4] are shown in figures 1(a-b) because these angles is dominated by the long range polarization and the short range static potential respectively as shown in figures1(a-b) also the interaction potentials as will as the relativistic correction according to the spin-orbit interaction term becomes more sensitive at low impact energies.As the incident energy increases my results agree well with the results of Nahar and Wadehra [4] except at the Ramsauer-Townsend minimum and maximum as shown in figure1(c-l),because the effects of the polarization,correlation and the exchange becomes negligible at high energies, only the static potential dominate ,where the static potential used in this work is completely determined by the adopted nuclear and electronic charge-density models which is differ from that used by Nahar and Wadehra [4].Also The correlation–polarization potential models considered in this work combine empirical information (static polarizability) with the local-density approximation (i.e. the target is regarded as a locally homogeneous electron gas),while Nahar and Wadehra [4] they had been used only polarization potential without correlation potential for the short and long range limit.

4. Conclusions

The elastic scattering of electrons from argon atom has been treated relativistically by solving the Dirac equation numerically for the model potential representing the projectile-target interaction which is consist of Static,Exchange and Correlation-Polarization terms.I take the exchange potential to include it in the total scattering potential model because of exchange effects are due to the Pauli exclusion principle,consequently, exchange potential prevent two electrons of like spin from being found near one another because it make each bound electron is surrounded by a “ Fermi hole” where the repulsive Coulomb interaction between two electrons of like spin vanishes .Also , i included the correlation potential in the total scattering potential model because each electron is assumed to move in the average self consistent field of other electron,taking in to account only the Coulomb energy and the Pauli exclusion principle .Thus, the correlation potential is the correction of this average interaction to allow electrons to avoid one another ,not only “ on the average’ but in every region of configuration space .Thus in addition to the “ Fermi hole” caused by the exchange potential ,the correlation potential make each electron surrounds itself with a “ Coulomb hole” from which other electrons are excluded when a single electron is removed sufficiently far from the other electrons .These effects are important for argon atom as will as other atomic systems except for hydrogen atom where there is one electron in this atom.Therefore ,if these effects are neglected ,then the results obtained does not have any physical feature .The calculated values of spin polarization parameter $S(\theta)$ in the energy range of 3-300eV agree reasonably well with the available theoritical values except at low energies ($\leq$ 5 eV) because of the long range polarization and the short range static potential respectively as will as the relativistic correction terms according to the spin-orbit interaction becomes more sensitive at low impact energies. As the incident energy increases my results agree well with the other results because the effects of the polarization,correlation and the exchange becomes negligible at high energies,where only the static potential dominate.The dependence of the electron exchange,correlation and polarization potentials on the radial distance, according to the relativistic terms in the Dirac equation, becomes more important at low energies.

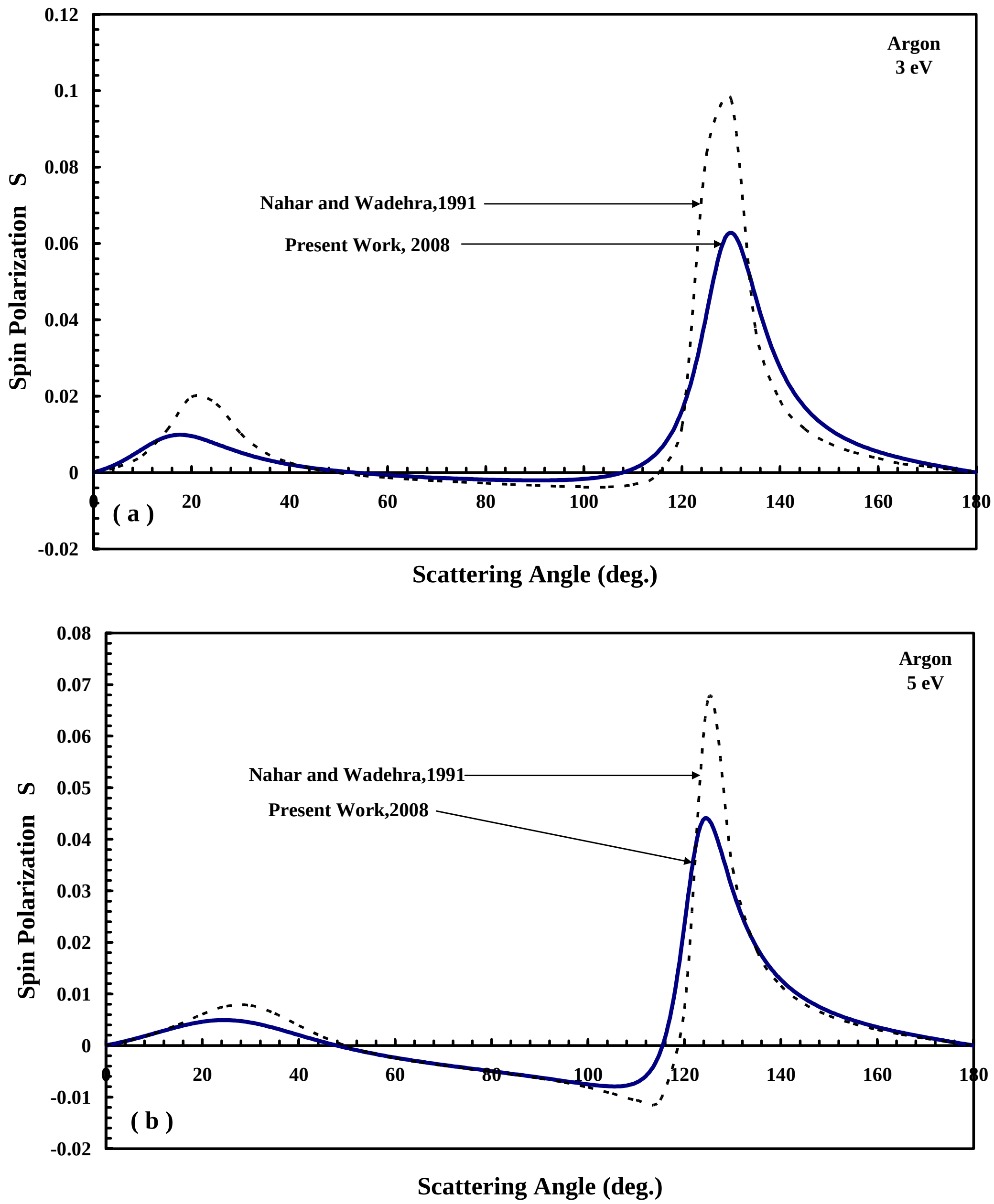


Figure (1) : Spin Polarization $S(\theta)$ for the elastic scattering of electrons from argon atoms for an incident electron energy (a) 3 eV, (b) 5 eV,(c) 10 eV , (d) 15 eV , (e) 20 eV , (f) 30 eV , (g) 50 eV , (h) 75 eV , (i) 100 eV , (j) 150 eV , (k) 250 eV and (l) 300 eV ,in all energies the solid curve corresponds to results obtained in present work,while the dotted curve corresponds to results obtained by Nahar and Wadehra (ref.[4]).

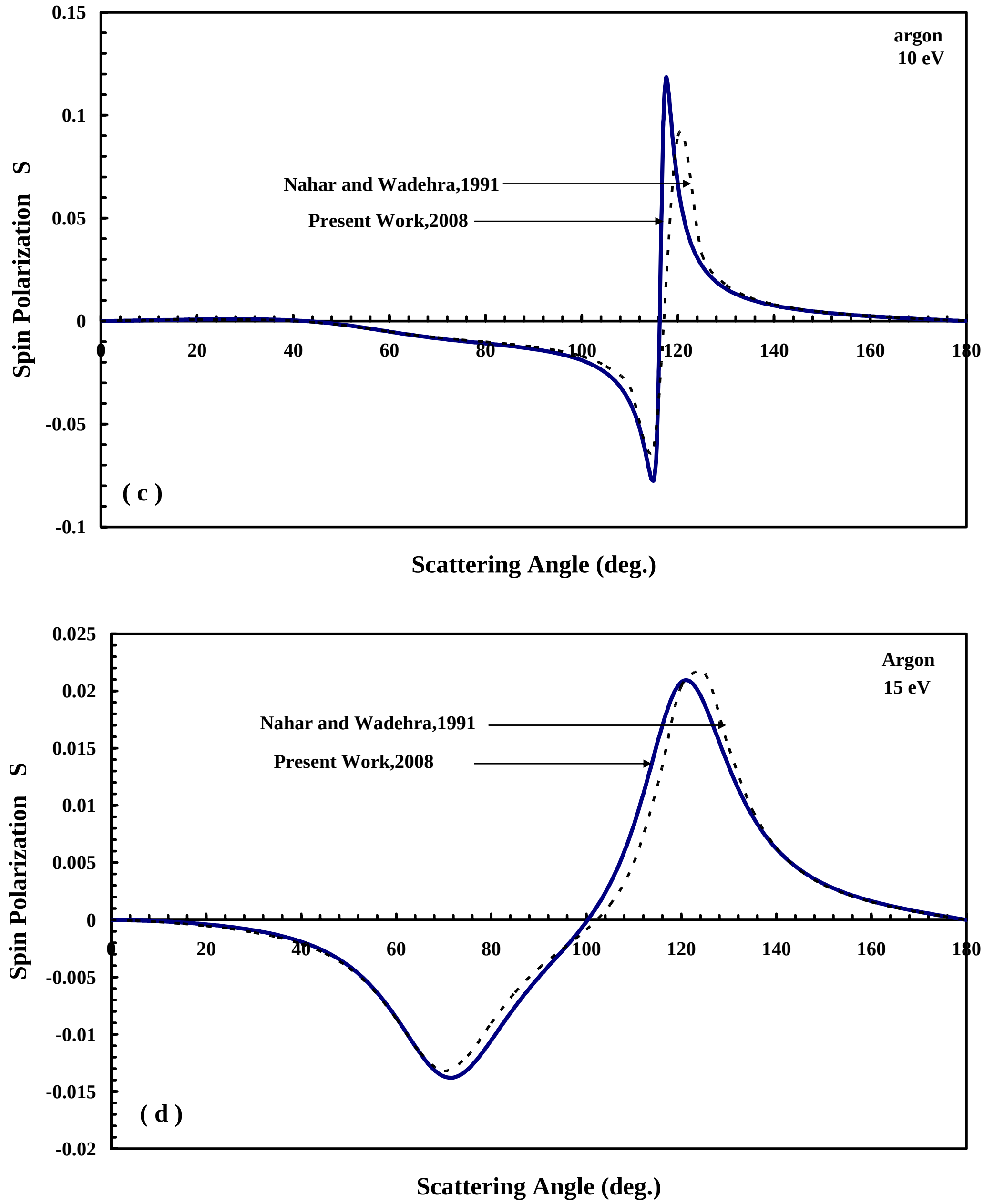
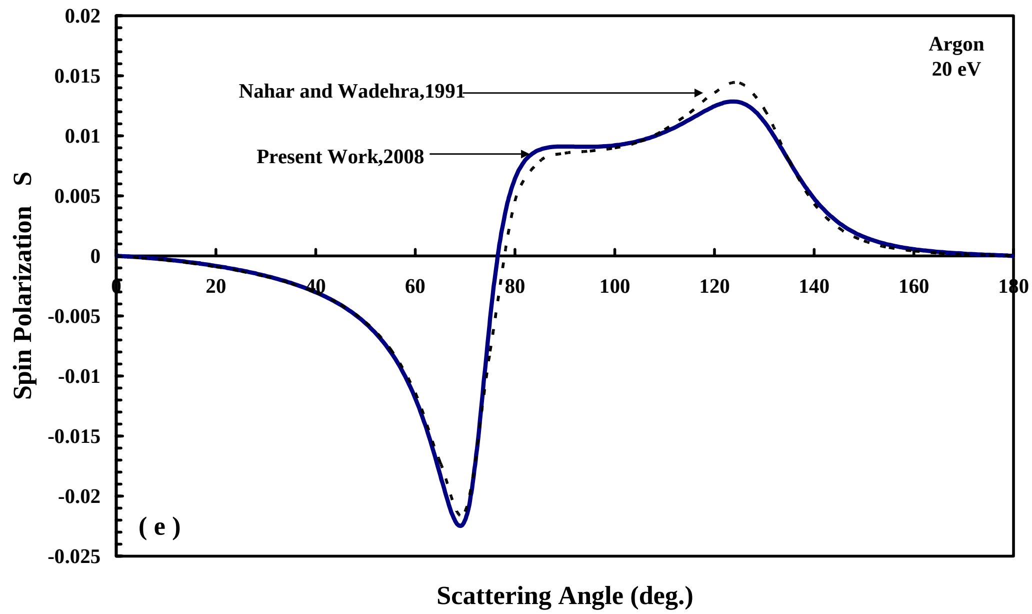


Figure (1).


Argon
20 eV
Nahar and Wadehra,1991
Present Work,2008
Spin Polarization S
Scattering Angle (deg.)
(e)

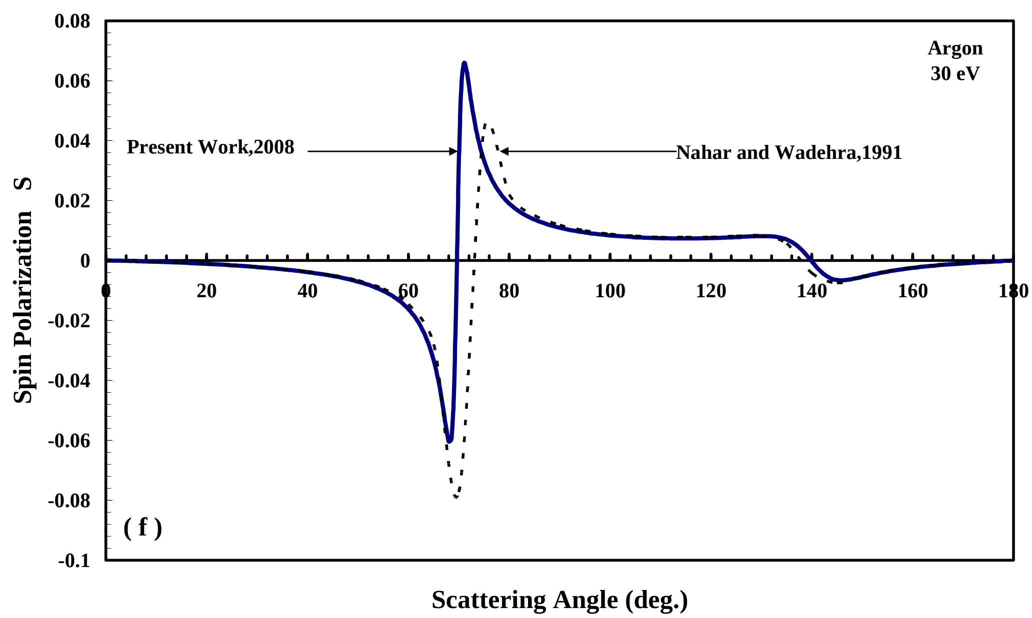
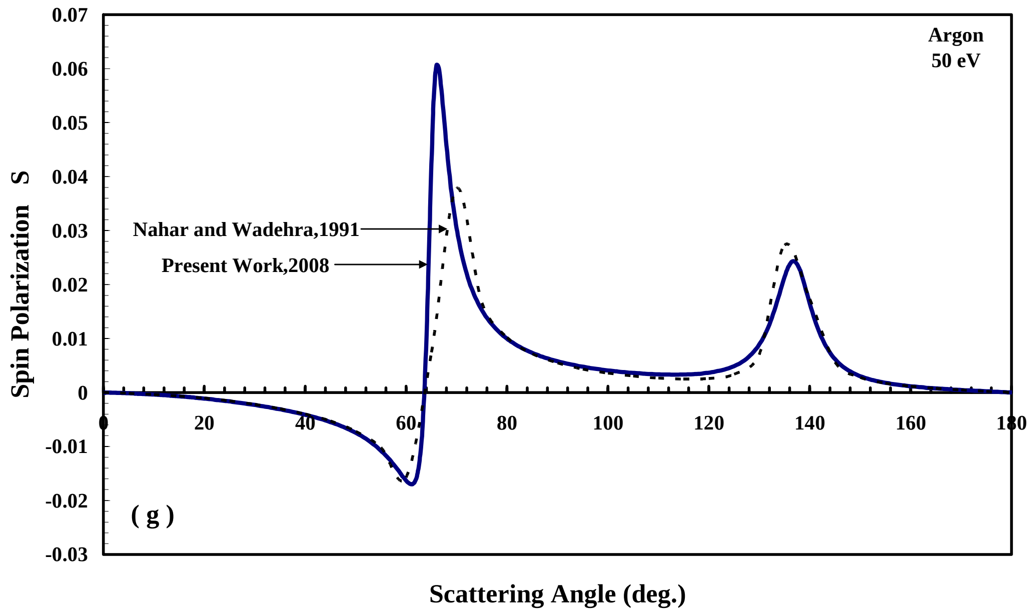

Argon
30 eV
Present Work,2008
Nahar and Wadehra,1991
Spin Polarization S
Scattering Angle (deg.)
(f)

Figure (1).


Argon
50 eV
Nahar and Wadehra,1991
Present Work,2008
(g)
Spin Polarization S
Scattering Angle (deg.)

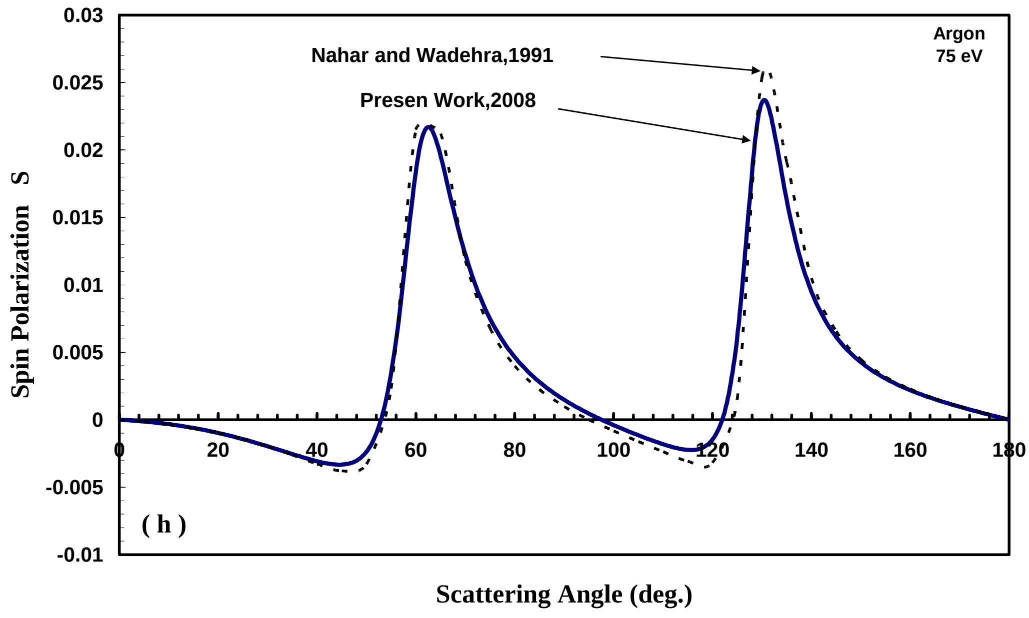
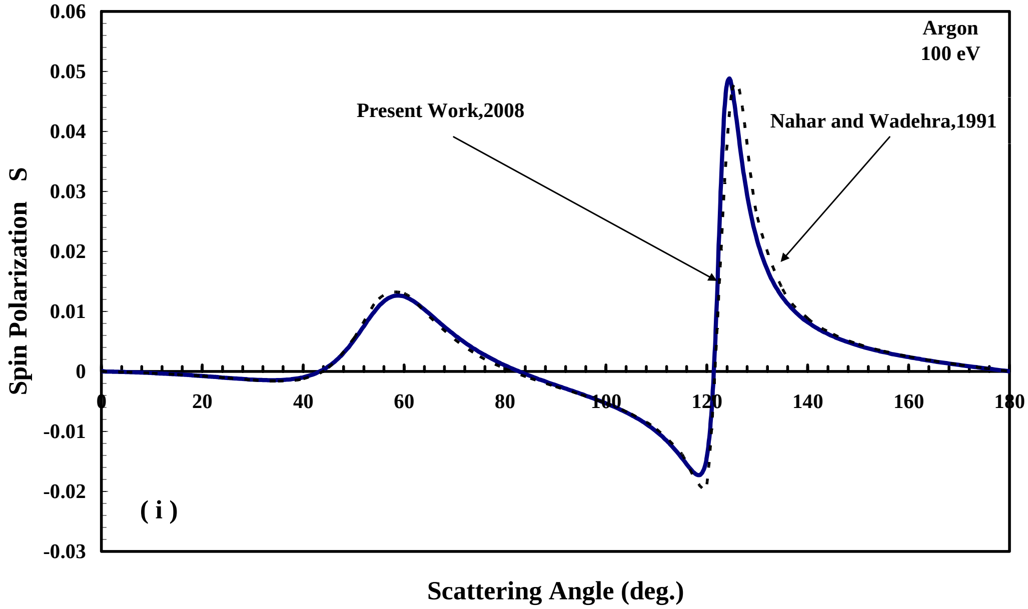
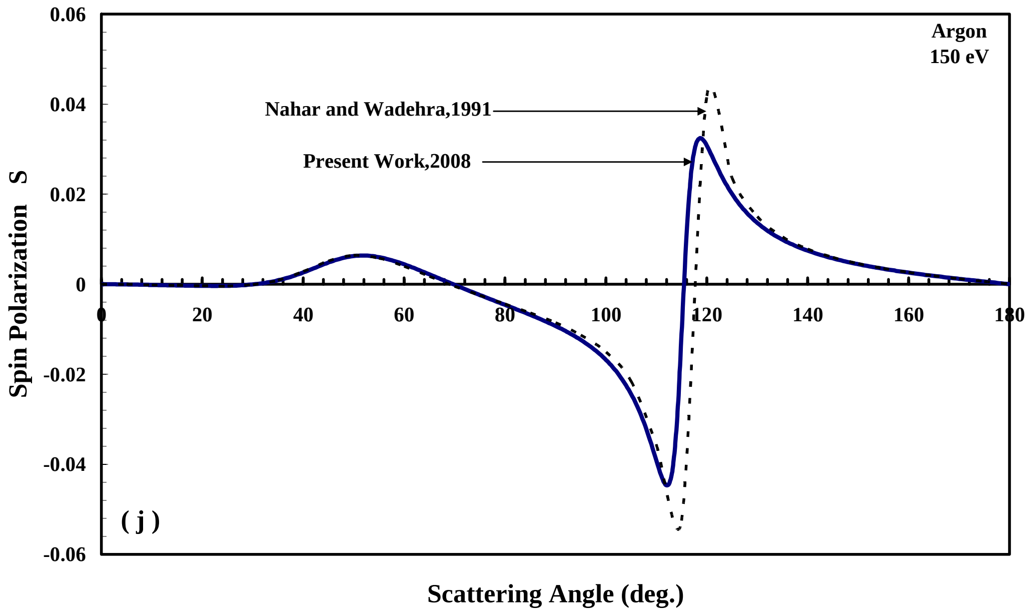

Argon
75 eV
Nahar and Wadehra,1991
Presen Work,2008
(h)
Spin Polarization S
Scattering Angle (deg.)

Figure (1).


Argon
100 eV
Present Work,2008
Nahar and Wadehra,1991
Spin Polarization S
Scattering Angle (deg.)
(i)
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
0
20
40
60
80
100
120
140
160
180


Argon
150 eV
Nahar and Wadehra,1991
Present Work,2008
Spin Polarization S
Scattering Angle (deg.)
(j)
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
0
20
40
60
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100
120
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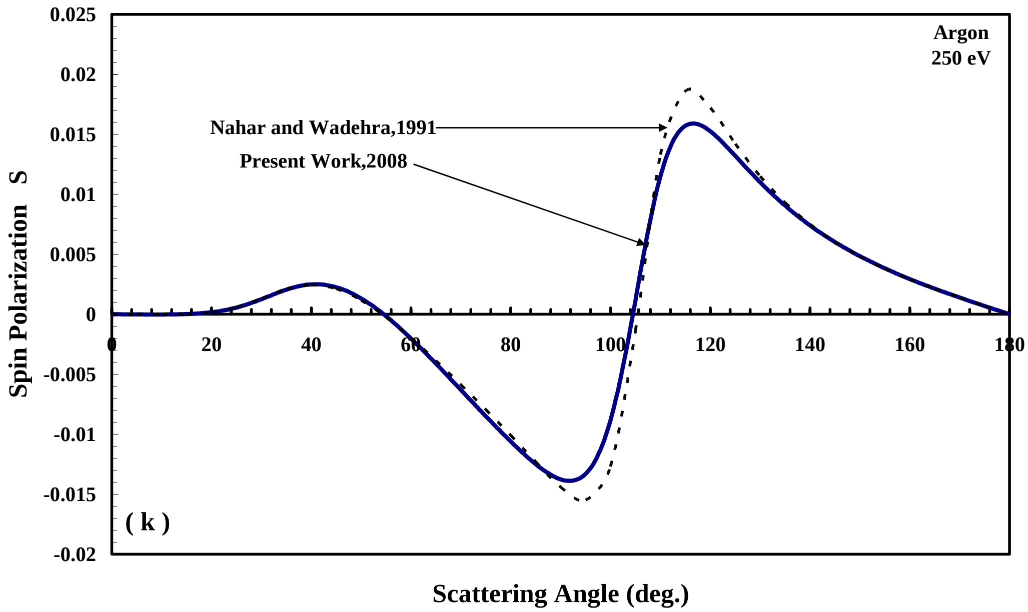
Figure (1).


Argon
250 eV
Nahar and Wadehra,1991
Present Work,2008
(k)
Spin Polarization S
Scattering Angle (deg.)

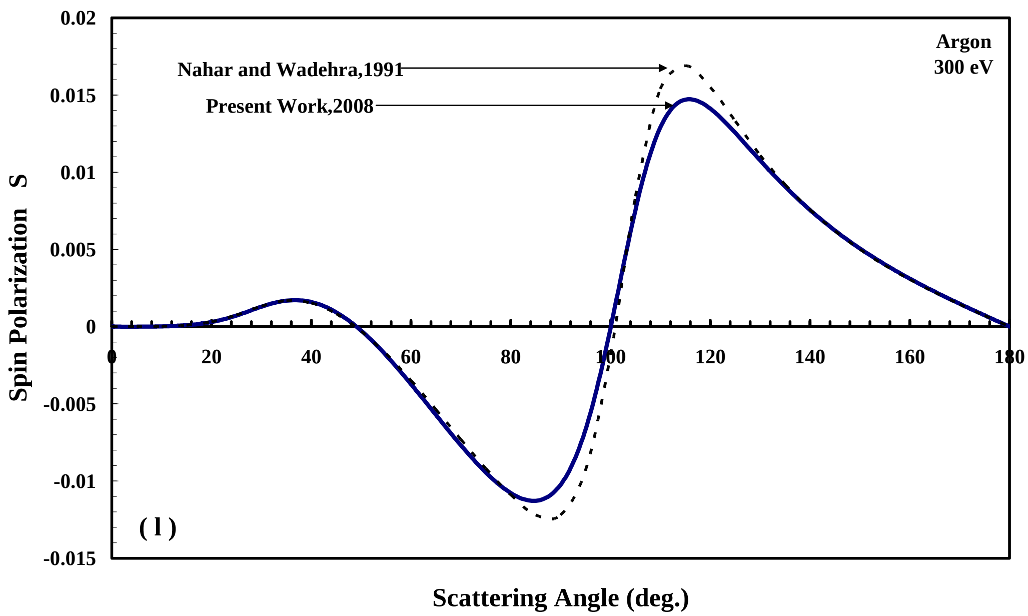

Argon
300 eV
Nahar and Wadehra,1991
Present Work,2008
(l)
Spin Polarization S
Scattering Angle (deg.)

Figure (1).

References

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