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Spin polarization for electrons scattering from cadmium and mercury atoms

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Abstract

Spin polarization parameter or the so –called Sherman function for the scattering of electrons from cadmium atom in the energy range of 6.4300 eV and mercury atoms in the energy range of 1- 14 eV are calculated using the relativistic Dirac equation .The projectile-target interaction is represented by an optical potential which consists of a sum of model potentials in the solution of relativistic Dirac equation .The results obtained for the spin polarization parameter are found to be in good agreement with the available calculations.

Keywords: Relativistic; Electron Scattering; cadmium and mercury atoms; Dirac Equation ; Spin Polarization.

1.Introduction:

Theoretical studies of spin-dependent phenomena in collisions between electrons and atoms have progressed significantly since the classic review of Kessler [1].It is well known that the relativistic interaction plays an important role in understanding this phenomenon in the scattering of electrons from heavy atomic targets. The relativistic approach, start 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. The spin polarization of electrons during scattering by a central field was first investigated by Mott [4],using a relativistic treatment based on the theory of Dirac[5]. A few investigations have been made of electrons scattering from cadmium to obtain the scattering features of this comparatively

heavy atom (*Z=48*)[2,3].In the present work, the investigation performed on the same scattering problem using the calculations start with the Dirac equation to describe the scattering system and calculate the Spin polarization parameter S according to scattering in the impact energy range of (6.4-300 eV) for cadmium atom and (1-14 eV) for mercury atom .The relativistic treatment of electron collisions enables us to calculate the asymmetry function or the so- called Sherman function, which describes the calculated either left-right or spin-up and spin down asymmetries in the number of scattered electrons.

In sec.2 ,the computational method used in this paper, the calculated spin polarization parameter and the total interaction between an electron and a target atom are described. 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 projectile of rest mass m_o traveling in a central field $V(r)$ at a velocity *v* is given by[6]:

$$\left[c\alpha.P + \beta m_o c^2 + V(r)\right]\Psi = E\ \Psi \qquad (1)$$

Where $E = m_o\gamma c^2 = E_i + m_o c^2$ is the total energy, $\gamma = (1 - v^2/c^2)^{-1/2}$,and E_i is the kinetic energy of the incident particle. α and β are the usual 4 X 4 Dirac matrices. The spinor Ψ has the four components and Ψ = $(\psi_1,\psi_2,\psi_3,\psi_4)$,where $(\psi_1,\psi_2)$are large components and $(\psi_3,\psi_4)$are small components of ψ.For a central potential, the Dirac equation can be reduced to a set of two equations [7]:

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

Where $g_l^{\pm}$ is related to the radial part $G_l^{\pm}$ of the large component of Ψ by :

$$G_l = \sqrt{\eta}\,\frac{g_l}{r}, \eta = \frac{[E - V(r) + m_o c^2]}{\hbar c},$$

$K^2 = \dfrac{(E^2 - m_o^2 c^4)}{\hbar^2 c^2}$ .The $U_l^{\pm}$ are the effective Dirac potentials which are given in atomic units $(m_o = e = \hbar = 1, 1/c = \alpha$,where α is the fine-structure constant) by [6]:

$$-U_l^{+}(r) = -2\gamma V + \alpha^2 V^2 - \frac{3}{4}\frac{(\eta')^2}{\eta^2} + \frac{1}{2}\frac{\eta''}{\eta} + \frac{(l+1)}{r}\frac{\eta'}{\eta} \qquad (3)$$

and,

$$-U_l^{-}(r) = -2\gamma V + \alpha^2 V^2 - \frac{3}{4}\frac{(\eta')^2}{\eta^2} + \frac{1}{2}\frac{\eta''}{\eta} - \frac{1}{r}\frac{\eta'}{\eta} \qquad (4)$$

Here, single and double primes denote the first and second derivatives with respect to *r*, respectively. It should be noted that the last term of $U_1^{\pm}$ in Equations (3) and (4)

$$\frac{1}{4m_o^2c^2}\frac{1}{r}\frac{\partial V(r)}{\partial r}\sigma.L \qquad (5)$$

corresponds to the two eigenvalues of the well-known spin-orbit interaction, one according to spin up and other according to spin down[8]:

Here , σ is related to spin *S* as σ =2*S* and the value of $\langle\ \sigma\ .\ L\ \rangle$ equals *l* for $j = l + 1/2$ and $-(l+1)$ for $j = l - 1/2$.The proper solution of Eq.(2) behaves asymptotically as[6]:

$g_l^{\pm}(K,r) = Kr[\,j_l(Kr) - \tan(\delta_l^{\pm})\eta_l(Kr)]$, when $r \to \infty$ (6)

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 :

$$\tan\delta_l^{\pm} = -\frac{(r+h)g_l^{\pm}(r)\,j_l[K(r+h)] - rg_l^{\pm}(r+h)\,j_l(Kr)}{rg_l^{\pm}(r+h)\eta_l(Kr) - (r+h)g_l^{\pm}(r)\eta_l[K(r+h)]} \qquad (7)$$

In the present calculation, the wave functions $g_l^{\pm}$ are obtained by numerical integration of Eq.(2) using Numerov's method. The two complex scattering amplitudes $f(K,\theta)$ (the direct amplitude) and $g(K,\theta)$ (the spin-flip amplitude) are defined as[9]:

$$f(K,\theta) = \frac{1}{2iK}\sum_{l=0}^{\infty}\{(l+1)[\exp(2i\delta_l^{+}) - 1] + l[\exp(2i\delta_l^{-} - 1)]\}P_l(\cos\theta) \qquad (8)$$

And

$$g(K,\theta) = \frac{1}{2iK}\sum_{l=1}^{\infty}[\exp(2i\delta_l^{-}) - \exp(2i\delta_l^{+})]p_l^1(\cos\theta) \qquad (9)$$

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[7]:

$$\sigma_u(\theta) = \frac{d\sigma}{d\Omega} = |f|^2 + |g|^2 \qquad (10)$$

And the spin polarization parameter $S(\theta)$ had the form[10]:

$$S(\theta) = \frac{i(fg^* - f^*g)}{\sigma_u(\theta)} \qquad (11)$$

The spin polarization (Sherman function) S describes the spin polarization parameter of the scattered electrons if the incident electron beam is unpolarized. The total interaction between an electron and a target atom is described 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 the polarization $V_{cpol}(r)$,potentials .These 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 is obtained by [11]:

$V_{st}(r) = Z_o e\varphi(r) = Z_o e[\varphi_n(r) + \varphi_e(r)]$ (12)

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 [11]:

$$\varphi_n(r) = e\left(\frac{1}{r}\int_0^r \rho_n(r')4\pi r'^2 dr' + \int_r^{\infty}\rho_n(r')4\pi r' dr'\right) \qquad (13)$$

And

$$\varphi_e(r) = -e\left(\frac{1}{r}\int_0^r \rho_e(r')4\pi r'^2 dr' + \int_r^\infty \rho_e(r')4\pi r' dr'\right) \quad (14)$$

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 [11]:

$$\chi(r) = \frac{r}{Ze}\varphi(r) \quad (15)$$

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

$$\rho_n(r) - \rho_e(r) = -\frac{1}{4\pi e r}\frac{d^2}{dr^2}[r\varphi(r)] = -\frac{Z}{4\pi r}\frac{d^2\chi(r)}{dr^2} \quad (16)$$

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

$$\rho_n(r) = \frac{\rho_o}{\exp[(r - R_n)/Z] + 1} \quad (17)$$

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, has used the most accurate electron densities available for free atoms which are obtained from self-consistent relativistic Dirac–Fock (DF) calculations [12].The same density $\rho_e(r)$ is used to obtain the electron exchange potential. In the present work, the exchange potential model of Furness and McCarthy [13]which is local approximation to the exchange interaction are used to perform the calculations and are given by:

$$V_{ex}(r) = \frac{1}{2}[E - V_{st}(r)] - \frac{1}{2}\{[E - V_{st}(r)]^2 + 4\pi a_o e^4 \rho_e(r)\}^{\frac{1}{2}} \quad (18)$$

Where E is the total energy of the projectile. For the correlation-polarization potential $V_{cpol}(r)$,a parameter-free polarization potential based on the correlation energy of the target atom is used. It has two components, the short-range $V_{SR}(r)$ and the long-range $V_{LR}(r)$ parts and are given by [6] :

$$V_{cpol}(r) = \begin{Bmatrix} V_{cor.}^{SR}(r) & , r < r_c \\ V_{pol}^{LR}(r) & , r \geq r_c \end{Bmatrix} \quad (19)$$

Here, r_c is the point where the two forms cross each other for thefirst time. The short - range form for electron scattering from atoms is based on the free electron gas exchange potential and is given by [14,15]:

$$V_{cor.}^{SR}(r) = \left[\frac{d}{d_o + d_1 r_s + r_s^2}\right]\cdot\left[\frac{c_3}{\sqrt{c_5}}\right] - \frac{r_s}{3}\left[\left\{\frac{d}{d_o + d_1 r_s + r_s^2}\right\}\cdot\left\{\frac{c_1\cdot c_2 - c_3\cdot c_4}{c_5}\right\} - \left\{\frac{d(d_o + 2r_s)}{(d_o + d_1 r_s + r_s^2)^2}\right\}\cdot\left\{\frac{c_3}{\sqrt{c_5}}\right\}\right] \quad (20)$$

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

$$c_1 = r_s^2 + e_4 r_s^{3/2} + e_5 r_s + e_6\sqrt{r_s} \quad (21)$$

$$c_2 = e_1 + \frac{e_2}{2\sqrt{r_s}} \quad (22)$$

$$c_3 = e_1 r_s + e_2 \sqrt{r_s} + e_3 \quad (23)$$

$$c_4 = 2 r_s + \frac{3 e_4 \sqrt{r_s}}{2} + e_5 + \frac{e_6}{2\sqrt{r_s}} \quad (24)$$

$$c_5 = \left(r_s^{\,2} + e_4 r_s^{3/2} + e_5 r_s + e_6 \sqrt{r_s} \right)^2 \quad (25)$$

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[11]:

$$V_{pol}^{LR}(r) = \frac{-\alpha_d e^4}{2(r^2 + d^2)^2} \quad (26)$$

Where (α_d) is the dipole polarizability of the target atom .For cadmium atom it is taken to be (43.7 a.u.) [2] and for mercury atom it is taken to be (44.84 a.u.)[16] , also the value of (d) is a phenomenological cut-off parameter that serves to prevent the polarization potential from diverging at r = 0,where it is given by the expression of Mittleman and Watson [17] as:

$$d^4 = \frac{1}{2}\alpha_d a_0 Z^{-1/3} b_{pol}^2 \quad (27)$$

Where a_0 is atomic unit assumed equal to one and b_{pol}^2 is an adjustable energy-dependent parameter which is given by [17]:

b_{pol}^2 = max {(E-50 eV)/(16 eV),1} (28)

So ,in this work the assumption is that the Buckingham potential, is given by Eqs.(26)-(28).

3.Results And Discussion:

In this work the values of the spin polarization $S(\theta)$ for scattering of electrons by :

a : cadmium atom: at various impact energies between (6.4-300eV) are calculated relativistically by using the interaction potential in the Dirac equation where the results are compared with the available theoretical values of S.N.Nahar [3] ,these results are shown in figure1(a-l).Where the calculated values of spin polarization parameter agree reasonably well with the available theoretical values of S.N.Nahar [3] except at low impact energies (≤ 10 eV),these differences between our results and the results of S.N.Nahar [3] are shown in figures1(a-b) because the interaction potentials as well as the relativistic correctic according to the spin-orbit interaction term become more sensitive at low impact energies. As the incident energy increases our results agree well with the results of S.N.Nahar [3] except at the Ramsauer-Townsend minimum and maximum as shown in figure1(c-l),because the effects of the polarization, correlation and the exchange become 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 differ from these used by S.N.Nahar [3] .Also The correlation–polarization potential models considered in this work combine empirical information (static polarizability and an adjustable energy-dependent parameter) with the local-density approximation (i.e. the

target is regarded as a locally homogeneous electron gas),while S.N.Nahar [3] has used only the polarization potential without correlation potential for the short and long range limit.

b: mercury atom : the impact energies between (1-14 eV) are calculated by using the same optical potential in the Dirac equation where the results are compared with the available theoretical values of Szrnytkowski and Sienkiewicz [16].These results are shown in figure 2 (a-j) where the calculated values of spin polarization parameter agree reasonably well with the available theoretical values of Szrnytkowski and Sienkiewicz [16] as shown in fig 2(a-e).The small difference between the shape of the Sherman function of the present calculation and the shape of the Sherman function of Szrnytkowski and Sienkiewicz [16] at these impact energies because of the interaction potentials as well as the relativistic correction according to the spin-orbit interaction term becomes more sensitive at low impact energies. Also there is a difference between the present results and the results of of Szrnytkowski and Sienkiewicz [16] in the shape of the Sherman function at impact energies (6-14eV), as shown in fig2(f-j), because the effects of the polarization, correlation and the exchange become very small when impact energy increases where only the static potential becomes dominate ,where the static potential used in this work is completely determined by the adopted nuclear and electronic charge-density models which differ from the relativistic static potential used by Szrnytkowski and Sienkiewicz [16].Also the correlation–polarization potential models considered in this work combine empirical information (static polarizability and an adjustable energy-dependent parameter) with the local-density approximation (i.e. the target is regarded as a locally homogeneous electron gas),while Szrnytkowski and Sienkiewicz [16] they had used only relativistic polarization potential within the relativistic version of the polarized orbital approximation without correlation potential for the short and long range limit .

4. Conclusions:

The elastic scattering of electrons from cadmium and mercury atoms has been treated relativistically by solving the Dirac equation numerically for the model potential representing the projectile-target interaction which consists of Static, Exchange and Correlation-Polarization terms. We take the exchange potential to include it in the total scattering potential model because the exchange effects due to the Pauli exclusion principle, consequently, exchange potential that prevents two electrons of like spin from being found near one another because it makes each bound electron be surrounded by a " Fermi hole" where the repulsive Coulomb interaction between two electrons of like spin vanishes .Al the inclusion of the correlation potential in the optical scattering potential model because each electron is assumed to move in the average self consistent field of other electron, taking into 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 makes each electron surround itself with a " Coulomb hole" from which other electrons are excluded when a ingle electron is removed sufficiently far

from the other electrons .These effects are important for cadmium and mercury atoms as well as other atomic systems
especially when atomic number increases except for hydrogen atom where there is one electron in this atom. Therefore ,if these effects are neglected ,then the results obtained do not have any physical feature .The calculated values of spin polarization parameter $S(\theta)$ in the energy range of (6.4-300eV) for cadmium atom and (1-14 eV) mercury atom agree reasonably well with the available theoretical values except at low energies ($\leq$ 10 eV) because of the long range polarization and the short range static potential respectively as well as the relativistic correction terms according to the spin-orbit interaction that becomes more sensitive at low impact energies. As the impact energy increases our results agree well with the other results because of the effects of the polarization, correlation and the exchange become 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, become more important at low energies.

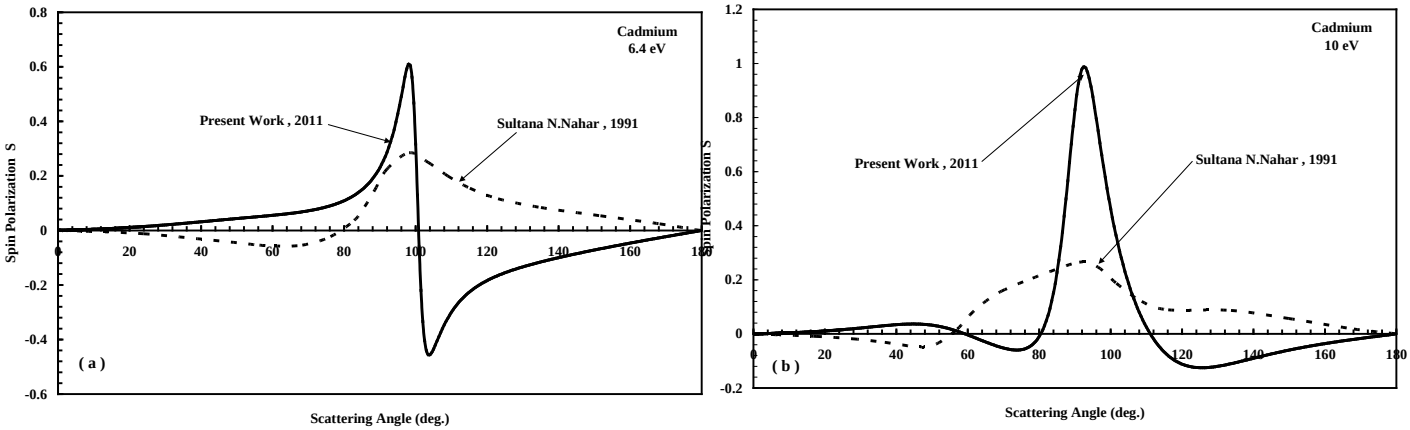
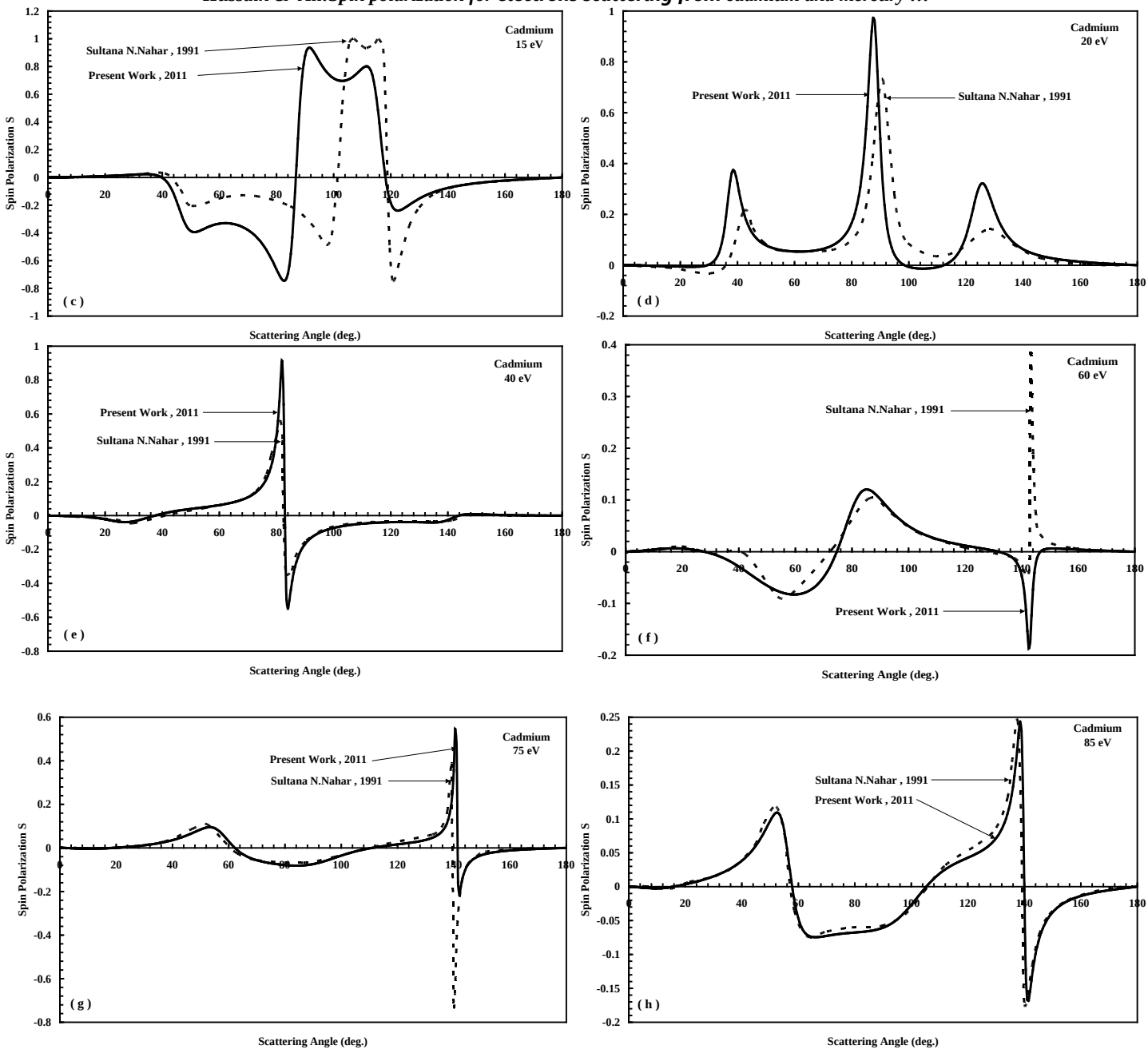
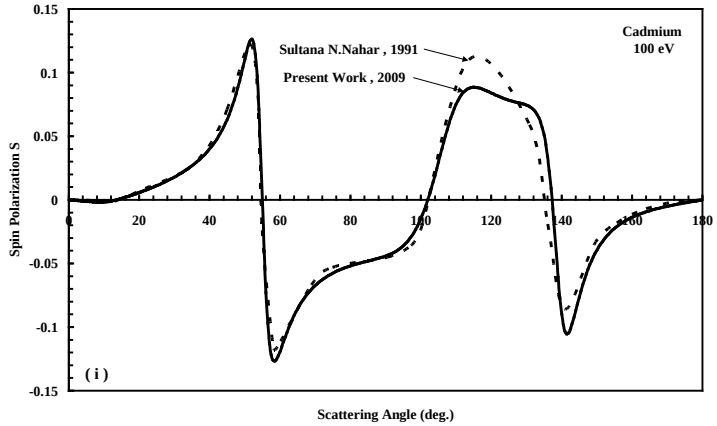
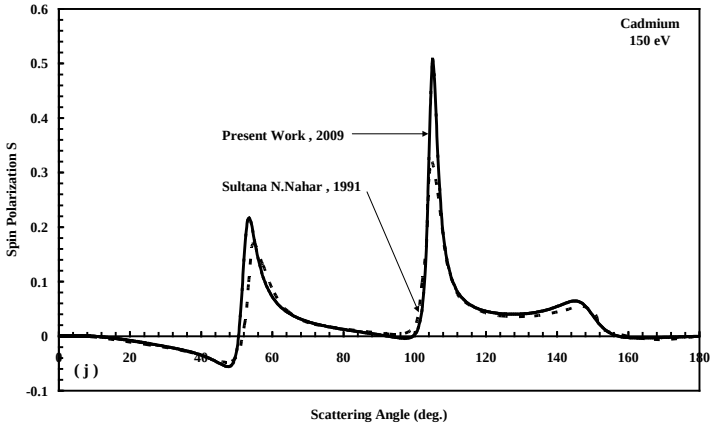
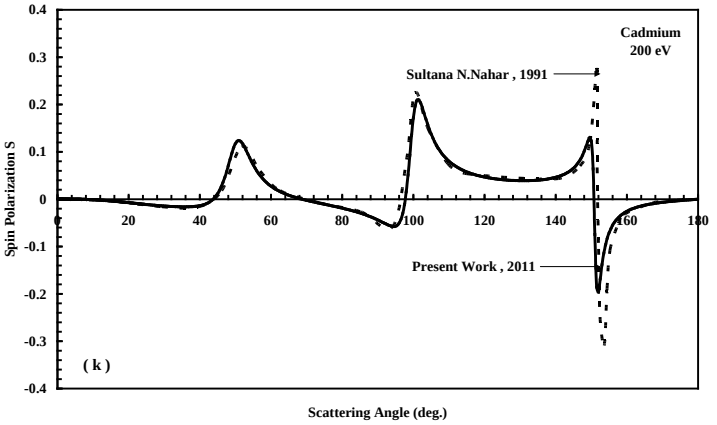


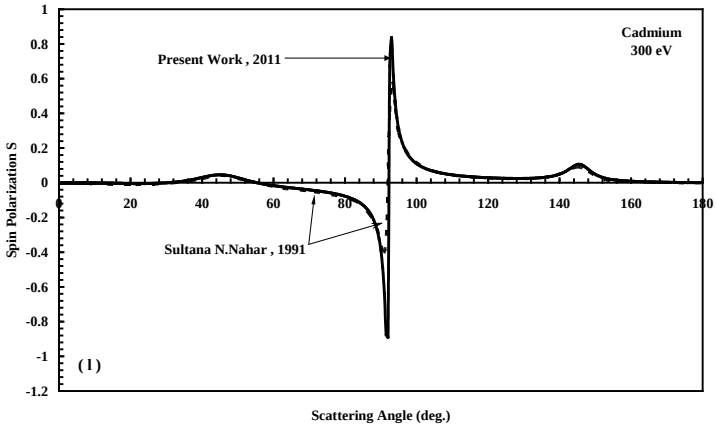
Figure (1) : Spin Polarization $S(\theta)$ for the scattering of electrons by cadmium atom for an impact energy (a) 6.4 eV, (b) 10 eV,(c) 15 eV , (d) 20 eV , (e) 40 eV , (f) 60 eV , (g) 75 eV , (h) 85 eV , (i) 100 eV , (j) 150 eV , (k) 200 eV and (l) 300 eV ,in all energies the solid curve corresponds to the results obtained in the present work, while the dotted curve corresponds to the results obtained by S.N.Nahar [2].

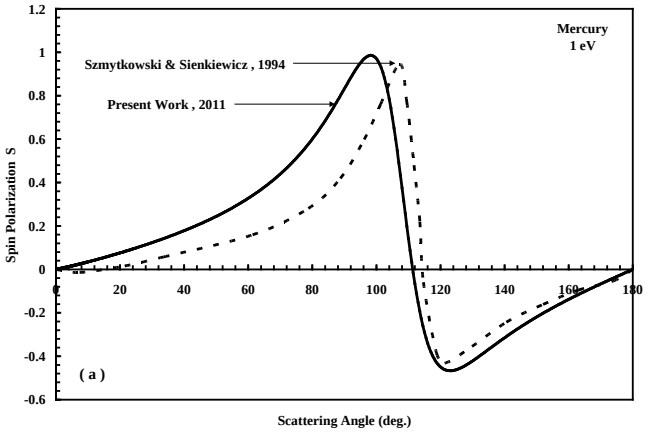

Cadmium
15 eV
Sultana N.Nahar , 1991
Present Work , 2011
(c)
Cadmium
20 eV
Present Work , 2011
Sultana N.Nahar , 1991
(d)
Cadmium
40 eV
Present Work , 2011
Sultana N.Nahar , 1991
(e)
Cadmium
60 eV
Sultana N.Nahar , 1991
Present Work , 2011
(f)
Cadmium
75 eV
Present Work , 2011
Sultana N.Nahar , 1991
(g)
Cadmium
85 eV
Sultana N.Nahar , 1991
Present Work , 2011
(h)
Spin Polarization S
Scattering Angle (deg.)

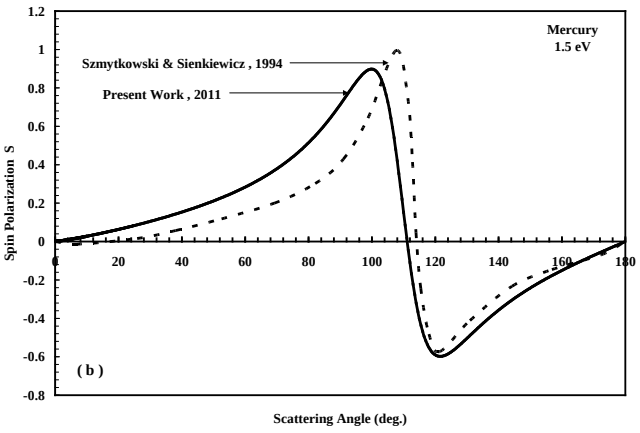

Cadmium
100 eV
Sultana N.Nahar , 1991
Present Work , 2009
Spin Polarization S
Scattering Angle (deg.)
(i)

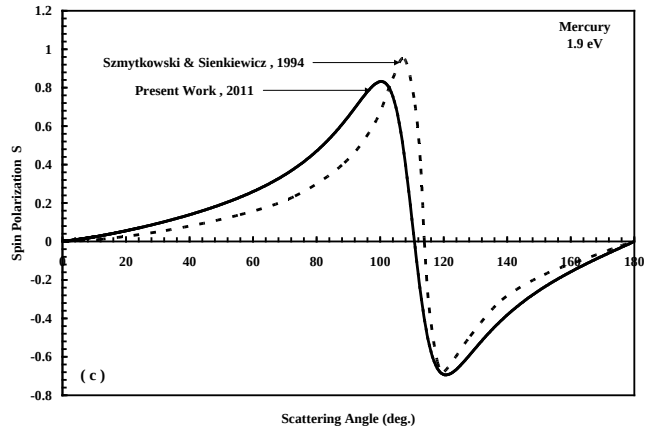

Cadmium
150 eV
Present Work , 2009
Sultana N.Nahar , 1991
Spin Polarization S
Scattering Angle (deg.)
(j)

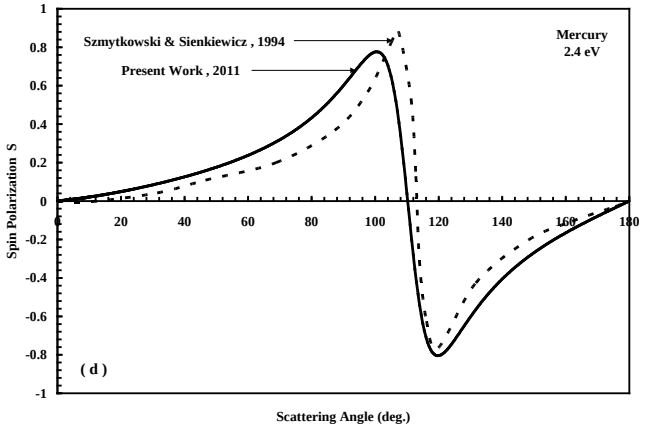

Cadmium
200 eV
Sultana N.Nahar , 1991
Present Work , 2011
Spin Polarization S
Scattering Angle (deg.)
(k)

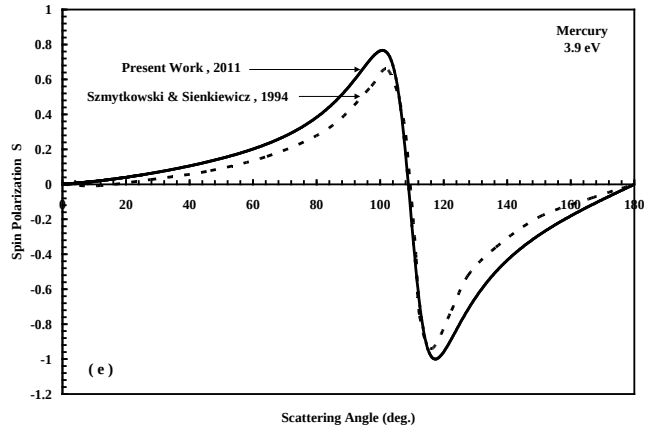

Cadmium
300 eV
Present Work , 2011
Sultana N.Nahar , 1991
Spin Polarization S
Scattering Angle (deg.)
(l)

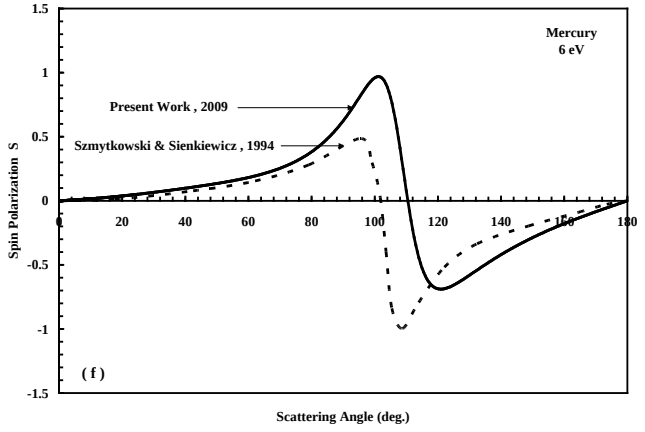

Mercury
1 eV
Szmytkowski & Sienkiewicz , 1994
Present Work , 2011
Spin Polarization S
Scattering Angle (deg.)
(a)

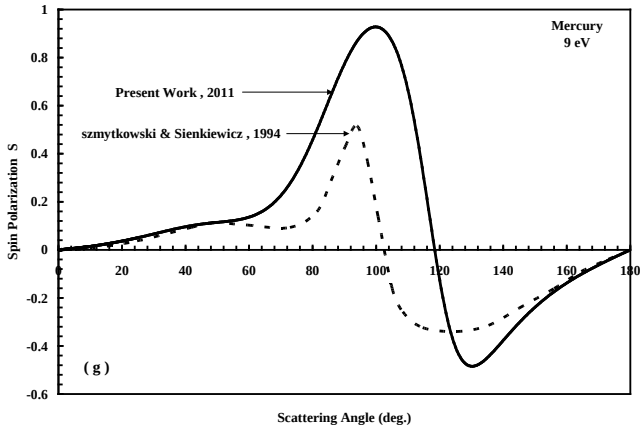

Mercury
1.5 eV
Szmytkowski & Sienkiewicz , 1994
Present Work , 2011
Spin Polarization S
Scattering Angle (deg.)
(b)

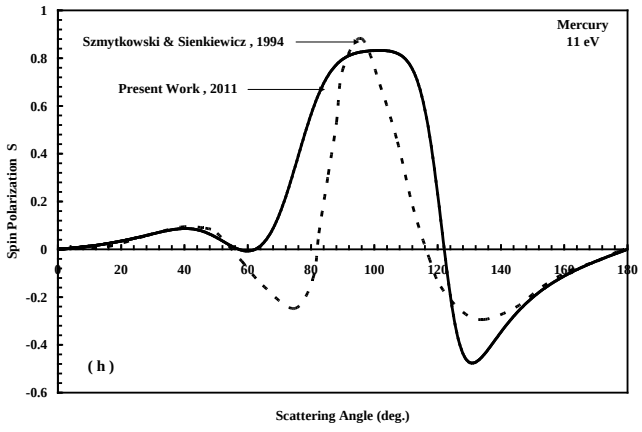

Mercury
1.9 eV
Szmytkowski & Sienkiewicz , 1994
Present Work , 2011
Spin Polarization S
(c)
Scattering Angle (deg.)


Mercury
2.4 eV
Szmytkowski & Sienkiewicz , 1994
Present Work , 2011
Spin Polarization S
(d)
Scattering Angle (deg.)


Mercury
3.9 eV
Present Work , 2011
Szmytkowski & Sienkiewicz , 1994
Spin Polarization S
(e)
Scattering Angle (deg.)


Mercury
6 eV
Present Work , 2009
Szmytkowski & Sienkiewicz , 1994
Spin Polarization S
(f)
Scattering Angle (deg.)


Mercury
9 eV
Present Work , 2011
szmytkowski & Sienkiewicz , 1994
Spin Polarization S
(g)
Scattering Angle (deg.)


Mercury
11 eV
Szmytkowski & Sienkiewicz , 1994
Present Work , 2011
Spin Polarization S
(h)
Scattering Angle (deg.)

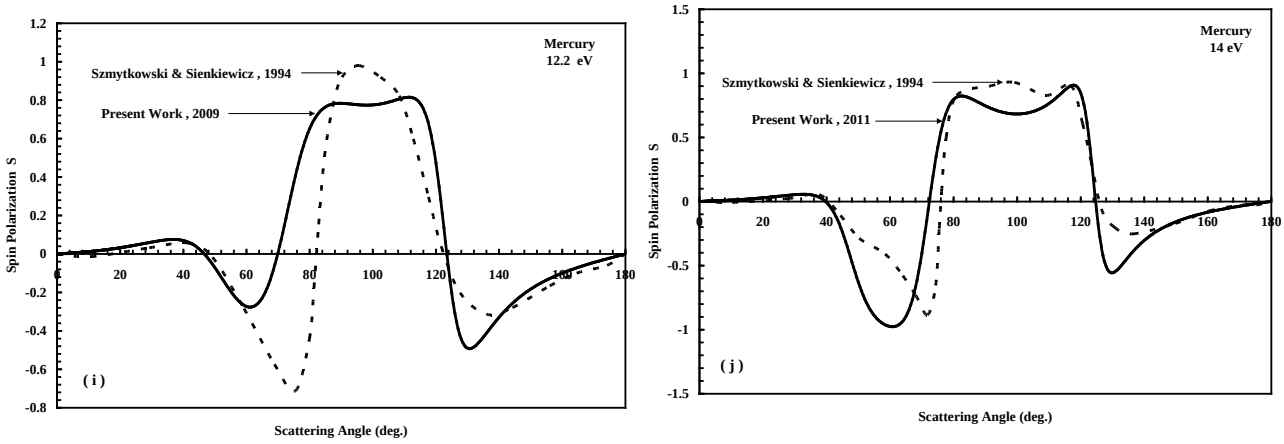


Figure (2) : Sherman function $S(\theta)$ for the scattering of slow electrons by mercury atom for an impact energy (a) 1 eV, (b) 1.5 eV,(c) 1.9 eV , (d) 2.4 eV , (e) 3.9 eV , (f) 6 eV , (g) 9 eV , (h) 11 eV , (i) 12.2 eV and (j) 14 eV, in all energies the solid curve corresponds to the results obtained in the present work, while the dotted curve corresponds to the results obtained by Szrnytkowski and Sienkiewicz [16].

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