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Relativistic Low-Energy Electron Scattering from Xenon Atoms

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Abstract:

Spin polarization has been calculated for the scattering of electrons from xenon atoms at impact energies up to 10 eV .The projectile-target interaction is represented by an optical potential used in the solution of relativistic Dirac equation . The calculations were carried out within a relativistic dirac method.Comparison with available results shows rather good agreement.

Keywords: Relativistic electron scattering ; xenon atom ; Dirac equation ; spin polarization.

1.INTRODUCTION:

Theoretical studies of spin-dependent phenomena in collisions between electrons and atoms have been 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.In the present work , the investigation is performed on the xenon target 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. 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 at low impact energies up to 10 eV. The relativistic treatment of electron collisions enables us to calculate the asymmetry function or spin polarization function or the so-called Sherman function, which describes the calculated spin-up and spin-down asymmetries in the number of scattered electrons.

In sec.2 ,the theory used in this paper will be introduced , in which the computational method used in present work , the calculated spin polarization parameter and the total interaction between an electron and a target atom will be 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 [2]:

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

Where $E = m_o \gamma c^2 = E_i + m_o c^2$ is the total energy which is not full relativistic since the energy is low,so quasirelativistic treatment is more suitable. $\gamma = (1 - v^2/c^2)^{-1/2}$,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 $\Psi = (\psi_1, \psi_2, \psi_3, \psi_4)$,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 [3]:

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

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

$$G_l = \sqrt{\eta}\,\frac{g_l}{r},\ \eta = \frac{[E - V(r) + m_o c^2]}{\hbar c},\ K^2 = \frac{(E^2 - m_o^2 c^4)}{\hbar^2 c^2}$$

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

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

And

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

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 $U_l^{\pm}$ in Equations (3) and (4) corresponds to the two eigenvalues of the well-known spin-orbit interaction, one according to spin up and other according to spin down [4]:

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

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[3]:

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

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 :

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

In the present calculation,the wave functions $g_l^{\pm}$ are obtained by using Numerov's method of Eq.(2).The two complex scattering amplitudes $f(K,\theta)$ (the direct amplitude) and $g(K,\theta)$ (the spin-flip amplitude) are defined as[5]:

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

And

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

Where θ is the scattering angle and $P_l(\cos\theta)$ and $p_l^1(\cos\theta)$ are the Legendre polynomial and the associated Legendre functions, respectively.The elastic differential cross section for the scattering of the unpolarized incident electron beam is given by [3]:

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

And the spin polarization parameter $S(\theta)$ has the form[6]:

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

The 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 [7]:

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

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 [7]:

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

And

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

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, *χ(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 [7]:

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

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:

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

Where $\rho_n(r)$ is obtained by Fermi distribution as [7] :

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

Where $Z = t/(4\ln 3) = 0.546\times 10^{-13} cm$ and $t = 2.4\times 10^{-13} cm$ (the skin thickness) defined as the distance over which the density drops from 0.9 to 0.1 of its central value, also $R_n = 1.07\times 10^{-13} A^{1/3} cm$, 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 it has used the most accurate electron densities available for free atoms which are obtained from self-consistent relativistic Dirac–Fock (DF) calculations [8].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[9] which is local approximation to the exchange interaction is used to perform the calculations and is given by:

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

Where E is the total energy of the projectile.For the correlation-polarization potential $V_{cpol}(r)$,a parameter-free polarization potential is based on the correlation energy of the target atom which is used.It has two components, the short-range $V_{SR}(r)$ and the long-range $V_{LR}(r)$ parts and are given by [2] :

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

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 potential and is given by [10,11]:

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

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

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

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

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

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

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

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 [7]:

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

Where (α_d) is the relativistic dipole polarizability of the target atom . For xenon atom it is taken to be (27.31 a_o^3) [12].And the value of (d_Ω) 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 [13] as:

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

Where a_0 is atomic unit assumed equal to one and b_{pol}^2 is an adjustable energy-dependent parameter which is given by [13]:

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

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

3.RESULTS AND DISCUSSION:

In this work the values of the spin polarization or the so-called Sherman function $S(\theta)$ for the scattering of slow electrons by xenon atom at various impact energies between (2-10 eV) are calculated relativistically by using the optical potential in the Dirac equation where the results are compared with the available theoretical values of P.Syty et.al. [14] ,these results are shown in figure1(a-d),where the calculated values of spin polarization parameter agree reasonably well with the available theoretical values of P.Syty et.al. [14] as shown in fig1(a-d), the difference between the shape of the Sherman function of my calculation and the shape of the Sherman function of P.Syty et.al. [14] 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 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.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 P.Syty et.al. [14] they had used the relativistic multiconfiguration method where the correlation effects responsible for target polarization were treated in a relativistic configuration-interaction scheme that allows for dynamical effects.

4. Conclusions:

The elastic scattering of electrons from xenon atom has been treated relativistically by solving the Dirac equation. The projectile-target interaction consists of Static,Exchange and Correlation-Polarization terms.These terms are important for xenon atoms as well as the other atomic systems especially when the atomic number increases.The relativistic correction terms according to the spin-orbit interaction becomes more sensitive at low impact energies, where 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.

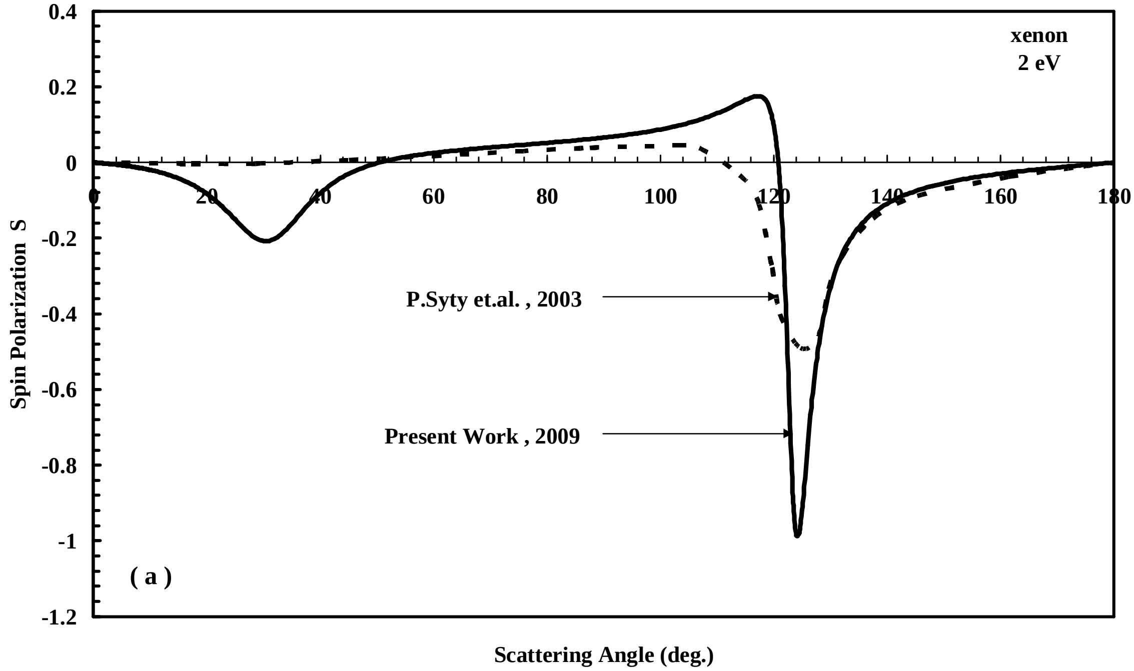
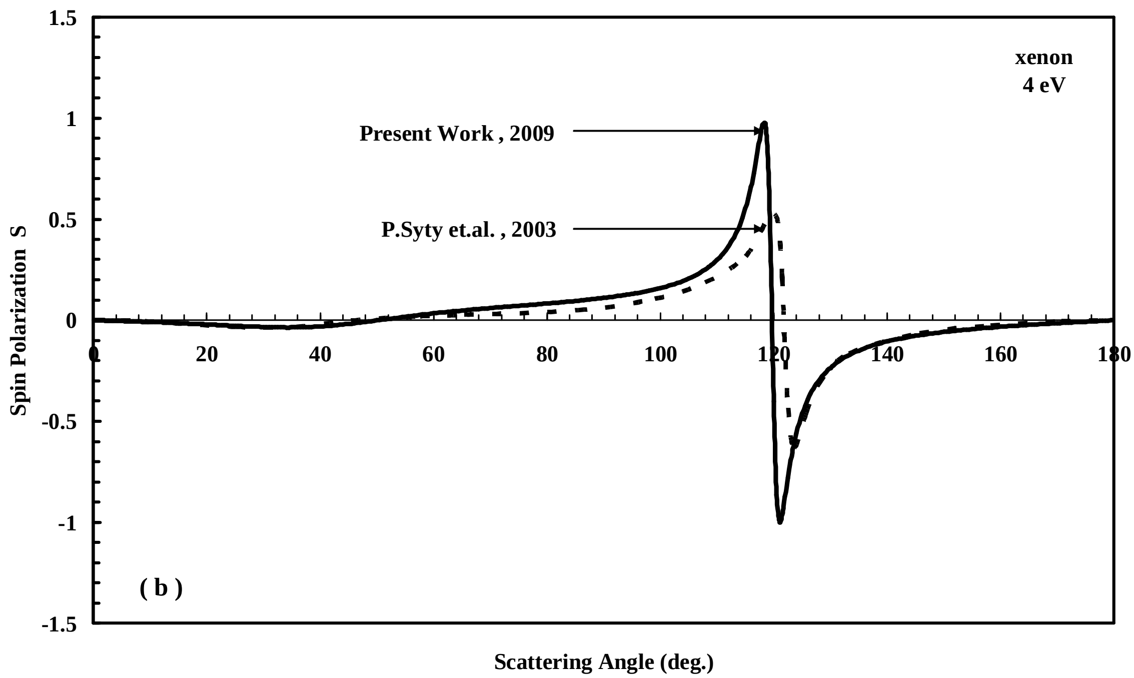


Figure (1) : Sherman function $S(\theta)$ for the scattering of slow electrons by xenon atom for an impact energy (a) 2 eV, (b) 4 eV,(c) 6 eV and (d) 10 eV, in all energies the solid curve corresponds to results obtained in present work, while the dotted curve corresponds to results obtained by P.Syty et.al. [14].



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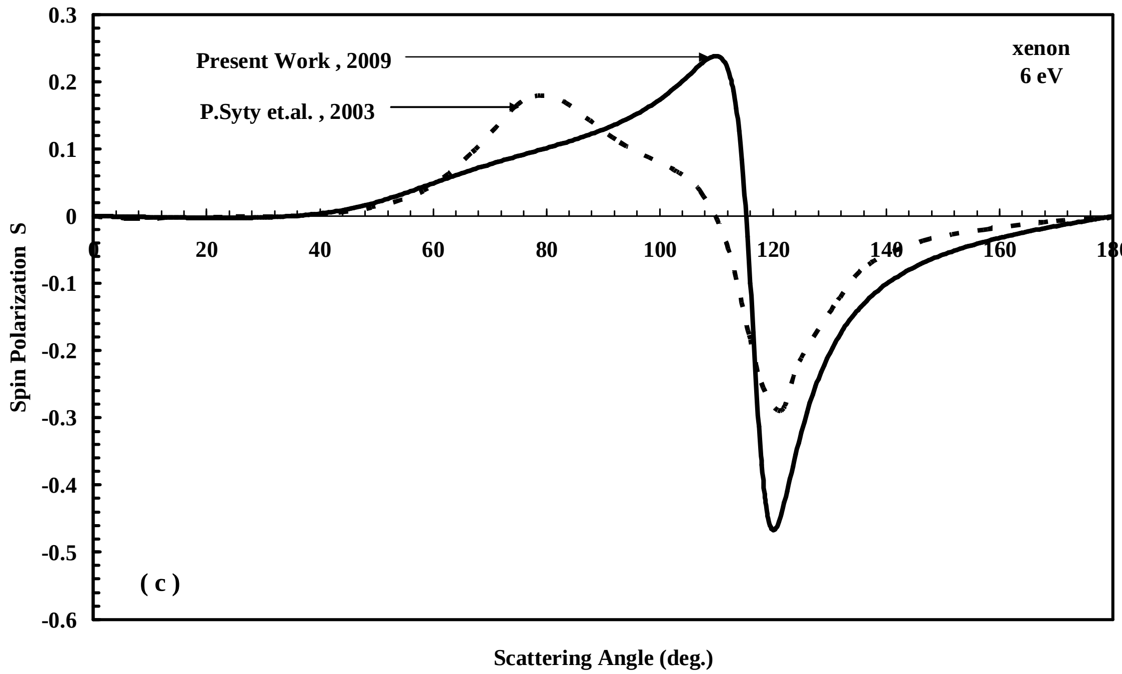

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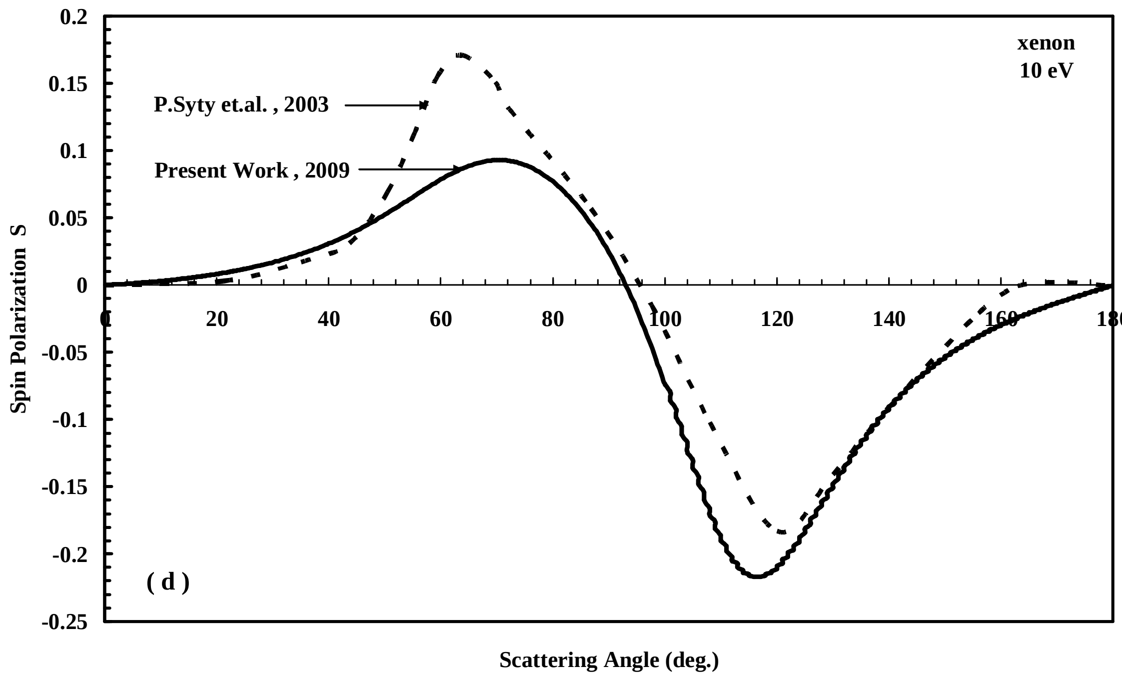

Figure (1). **continued**

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الاستطارة النسبية لالكترون الطاقة الواطئة من ذرات الزينون

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الخلاصة :

تم حساب استقطاب البرم لاستطارة الالكترونات من ذرات الزينون عند طاقات تصادم لحد 10 إلكترون فولت . إن تفاعل الجسيم المقذوف مع الهدف تم تمثيله بواسطة جهد بصري استخدم في حل معادلة ديراك النسبية. أنجزت النتائج باستخدام طريقة ديراك النسبية حيث إن مقارنة النتائج المنجزة بينت حالة اتفاق جيد نوعا ما مع النتائج المتوفرة .