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Relativistic Dirac Calculations for Electrons Scattering from Mg and Ca Atoms at Different Energies

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KEYWORDS:

- Relativistic
- Electron scattering
- Mg and Ca atoms
- Dirac equation
- Spin polarization

ABSTRACT

The cross sections of the electron scattering from atoms and spin polarization has been calculated for the scattering of electrons from Mg and Ca atoms at different energies using the relativistic Dirac equation. The interest of these calculations is to obtain an information about the scattering process. The incident electron- target interaction is represented by an a potential, which is consist of a sum of real model potentials used in the solution of relativistic Dirac equation. The comparison of the results obtained by this method are very good agreement with the other available results.

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حسابات ديراك النسبية لإستطارة الالكترونات من ذرات المغنيسيوم والكالسيوم عند طاقات مختلفة

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الكلمات المفتاحية:

- النسبية
- استطارة الإلكترون
- الذرات
- معادلة ديراك
- البرم

الـــخُـــلاصـــة

تم حساب المقاطع العرضية لاستطارة الالكترونات من الذرات وكذلك استقطاب البرم من ذرات المغنيسيوم والكالسيوم عند طاقات مختلفة بأستخدام معادلة ديراك النسبية، والاهتمام بهذه الحسابات للحصول على معلومات حول عملية الإستطارة، وتم تمثيل تفاعل الالكترون الساقط مع الهدف بجهد يتضمن مجموعة نماذج جهود أُستعملت لحل معادلة ديراك النسبية. وتمت مقارنة هذه النتائج مع النتائج المتوفرة لباحثين آخرين، وكان هناك توافق جيّد.

1. Introduction

The electron scattering from atoms is a fundamental atomic process in nature to obtain information about the structure and dynamics of astrophysical objects [1]. The cross sections of the electron scattering from atoms are needed in such different fields as astrophysics, atmospheric physics, plasma physics, and biophysics. Theoretical studies of relativistic effects and spin-dependent phenomena in collisions between electrons with atoms have been progressed significantly as given by the review of Kessler [1]. 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 are started with the Dirac equation to describe the scattering system and calculate the cross sections and Sherman functions according to scattering from Mg and Ca atoms at different incident energies. The relativistic treatment of electron collisions enables us to calculate the 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 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. Theoretical Part

The Dirac equation for the projectile of rest mass mo traveling in a central field at a velocity v is given by[2]:

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

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 $\Psi=(\psi^1,\psi^2,\psi^3,\psi^4)$, where (ψ^1,ψ^2) are large components and (ψ^3,ψ^4) are small components of ψ. For a central potential, the Dirac equation can be reduced to a set of two equations [3]:

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

Where, $g_l^{\pm}$ is related to the radial part $G_l^{\pm}$ of the large component of Ψ by [3] :

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

$$K^2=\frac{(E^2-m_o^2c^4)}{\hbar^2c^2}$$ .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]:

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

And

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

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 $U_l^{\pm}$ 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[3]:

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

Here, σ is related to spin *S* as $\sigma=2S$ and the value of $\langle\sigma\cdot L\rangle$ equals l for $j=l+\frac{1}{2}$ and $-(l+1)$ for $j=l-\frac{1}{2}$. The proper solution of Equation (2) behaves asymptotically as[4]:

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

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 $r+h(h \ll r)$ at very large r as [4] :

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

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

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

and

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

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]:

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

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

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

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 correlation 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]:

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

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]:

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

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, *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]:

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

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 [7] :

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

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

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

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,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 [7] :

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

Where E is the total energy of the projectile. For the correlation-polarization potential $V_{cpol}(r)$,

a parameter-free polarization potential is based on the correlation energy of the target atom which is used.It has two components, the short-range $V_{SR}(r)$ obtained from the local-density approximation by assuming that the correlation energy of the projectile at r is the same as if it were moving within a free-electron gas of density ρ_e equal to the local atomic electron density and the long-range $V_{LR}(r)$ parts and are given by [2] :

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

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 given by Perdew and Zunger [10], where the correlation potentialis given by [10]:

$$V_{COR}^{SR}(r) = \begin{bmatrix} -\frac{e^2}{a_o}(0.0311\ln(r_s) - 0.058 + 0.0013 r_s\, ln(r_s) - 0.0084 r_s) \;\; at \;\; r_s < 1 \\ -\frac{e^2}{a_o}\left(\frac{-0.1423-0.1748\sqrt{r_s}-0.0633 r_s}{(1+1.0529\sqrt{r_s}+0.3334 r_s)^2}\right) \quad at \quad r_s \geq 1 \end{bmatrix} \quad (20)$$

Where $r_S = \{3/[4\pi\rho_e(r)]\}^{1/3}$ is density parameter , $\rho_e(r)$ is the undistorted electronic density of the target.The long-range form of polarization potential is given by Buckingham model[7]:

$$V_{pol}^{LR}(r) = \frac{-\alpha_d e^4}{2(r^2 + d_\Omega{}^2)^2} \quad (21)$$

Where, (α_d) is the relativistic dipole polarizability of the target atom. For Mg atom it is taken to be ($10.06\times 10^{-24} cm^3$) and for Ca atom it is taken to be ($22.80\times 10^{-24} cm^3$) [11].The value of ($d_\Omega$)is a phenomenological cut-off parameter that servesto prevent the polarization potential from diverging at r = 0,

whereit is given by the expression of Mittleman and Watson [12] as:

$$d_{\Omega}{}^{4} = \frac{1}{2}\alpha_d a_0 Z^{-1/3} b_{pol}^2 \qquad (22)$$

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]:

$$b_{pol}^2 = \max\{(\text{E-50 eV})/(16\text{ eV}),1\} \qquad (23)$$

So ,in this work the assuming is that the Buckingham potential, is given by Eqs.(21)-(23)

3. Results and Discussion

In the present work, the relativistic Dirac method is used to calculate the scattering cross – sections, and momentum transfer cross sections of the electrons scattered by Mg and Ca- atoms by using the ELSEPA code of Salvat .et .al [7] Figure (1) shows the different incident energies for Mg–atoms at different incident energies (10,15,20,40,60,80,100,300) eV , our results were consistent with results of other investigators, the static effect is the dominant factor in the Scattering process, whereas the differences at low energies is due to the other limits of the efforts being included because the potential is sensitive to the incident electron energy especially at low energies ,also Figure (2) Shows the total cross sections (TCS's) for Mg- atoms ,Which is compared with theoretical calculation of Ismail et.al [14] and experimental measurements of Williams et. al [15] and predojevi et . al.[16], Where we did not agree with our results where it is observed at low energies, the value of these sections is great because the beam of electrons falling down affects the potential strongly at these energies. Figure(3) explains the momentum transfer cross sections from Mg - atoms, where no results were available to compare with them, but it was observed at high energies the Momentum transfer cross- sections decreases slowly as a function of the energy of the electron and potential . Figure (4) shows the differential cross – section from Ca- atoms for an incident electron energies (10 , 40, 60 , 200 , 300 , and 500) eV , our results are compared with the results of other investigators and were theoretically compatible with Hassan et.al. [17] , Pandya [18] and Khare [19] and experimental measurements of milisavljevic et. al. [20] .The DCSs can be greatest at the small angle because the beam of electrons falling close to the center of the control of central potential of the target.

Figure (5) also shows the total cross sections for electrons from Ca- atoms , where it these are a mismatch in the results and the difference in the potential used, also found in figure(6),that the momentum transfer cross sections for the scattering electrons from Ca– atoms. Also, we calculate the values of the spin polarization S(Θ) for scattering of electrons by two atoms , Magnesium atoms at various impact energies between (10-500) eV were calculated relatives tically by using the interaction potential in the Dirac equation , as show in Figure (7) , it was noted that there is a difference in the results due to the different incident energies, the effort of the reaction and the relative corrections applied to spin – orbit interaction (SOI) , as we not that limit is very sensitive at low energies, our results are the best,When the incident energy increases, we did not get the theoretical or experimental results to compare with our results .

Figure(8) explain the spin polarization parameters S,T,U at 10 eV for Scattering as shown in Figer (8) (a,b,c) and 200 eV of (d,e,f) by Mg-atoms ,also, Figures (9) shows the variation of Spin polarization parameters S(Θ) with scattering angle at incident energies(10 – 80) eV . for Ca – atoms . Figure (10) explains the spin polarization parameter S,T,U at 10 eV for Scattering of (a,b,c) and 200 eV of (d,e,f) by Ca -atoms .Our results calculated by this method are in very good agreement with other at all.

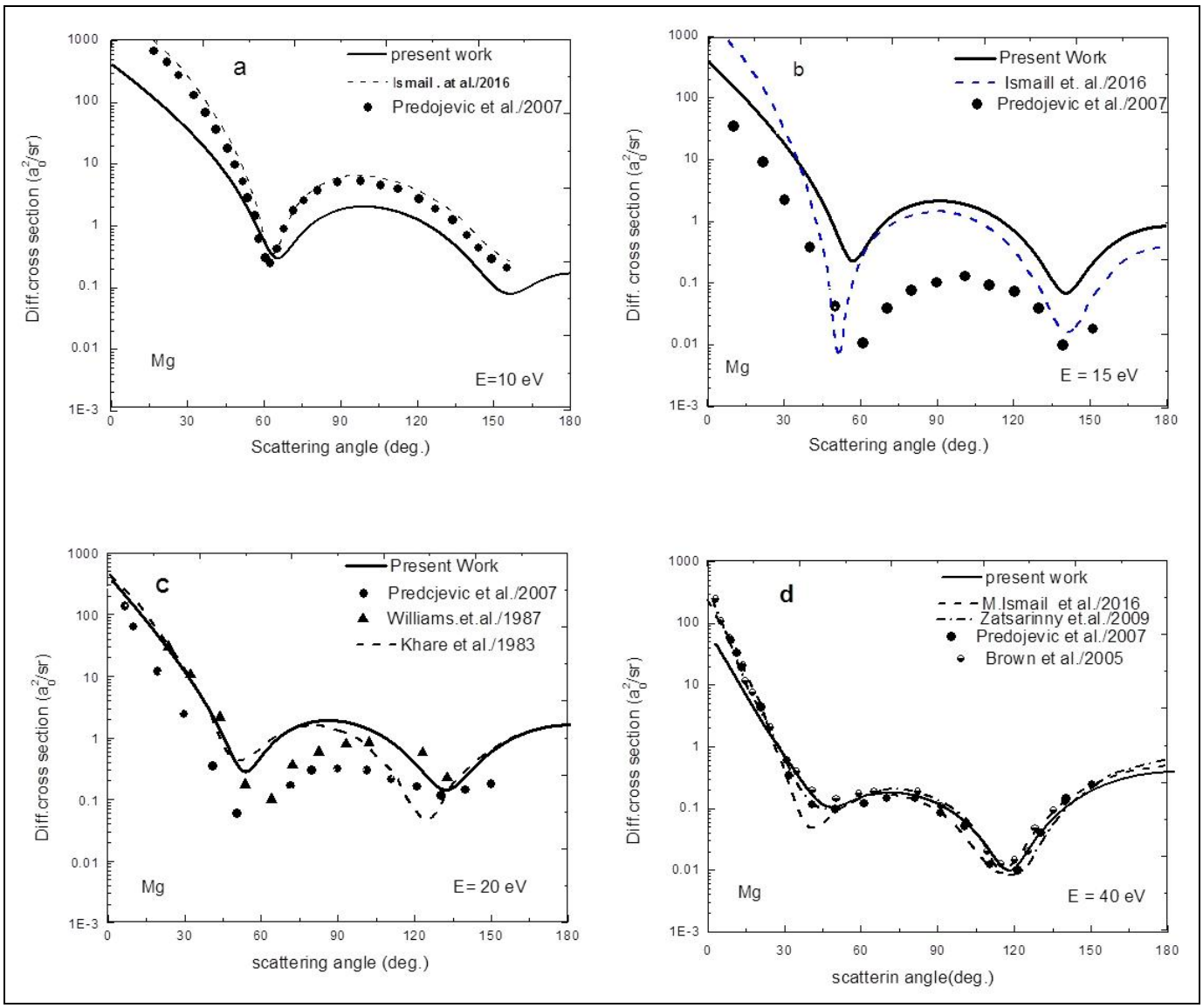


Figure (1): Differential cross-sections (a_0^2/sr) for the Scattering of electrons from Mg- atoms for an incident electron energy (a)10 eV ,(b)15 eV,(c) 20 eV , (d) 40 eV.

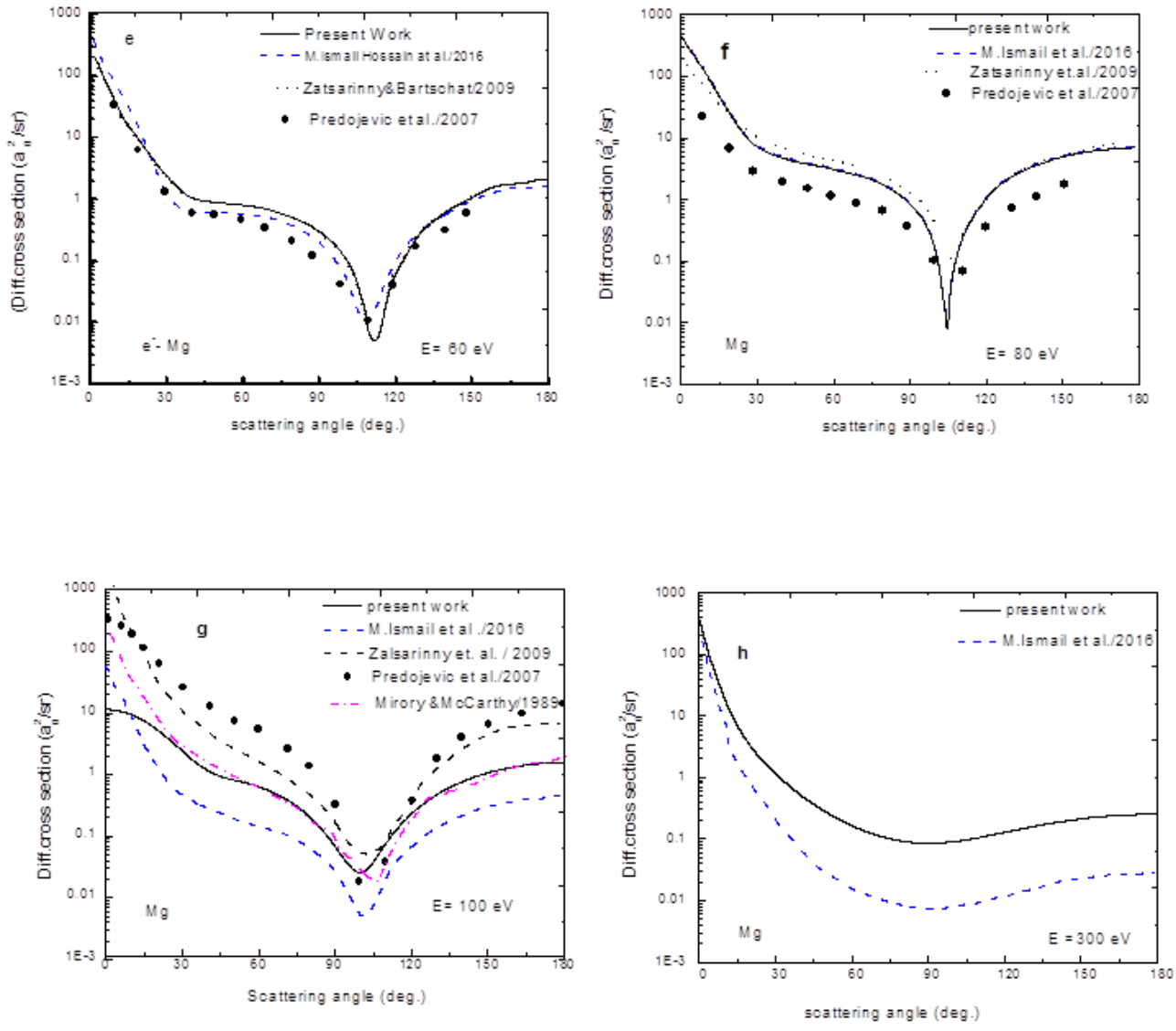
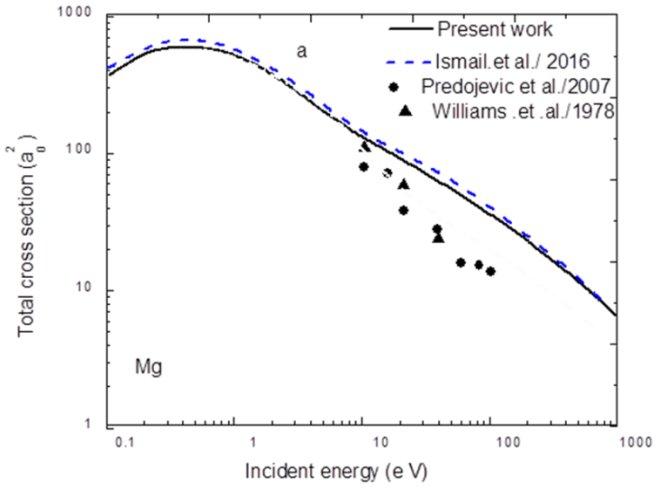


Figure (1): Differential cross-sections (a_0^2/sr) for the Scattering of electrons from Mg- atoms for an incident electron energy, (e) 60eV, (f)80 eV, (g)100 eV, (h) 300eV.



Figur (2): Total Cross – Sections(a20) for the Scattering of electrons from Mg- atoms in the incident electron energy range (1-1000) eV.

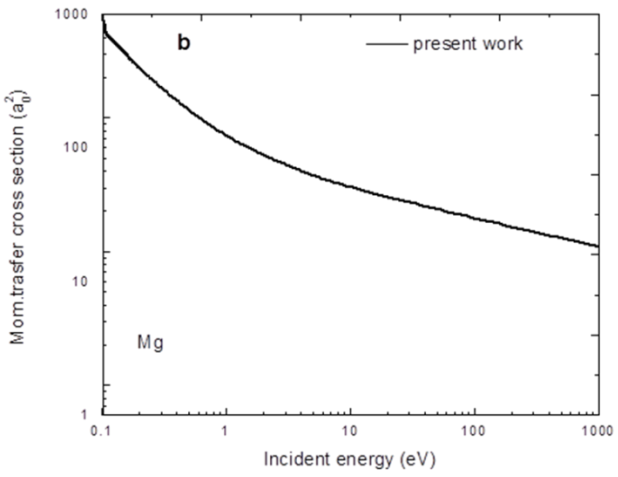


Figure (3): Momentum transfer cross-sections (a02) for the scattering of electrons Mg-atoms in the energy range (1- 1000) eV.

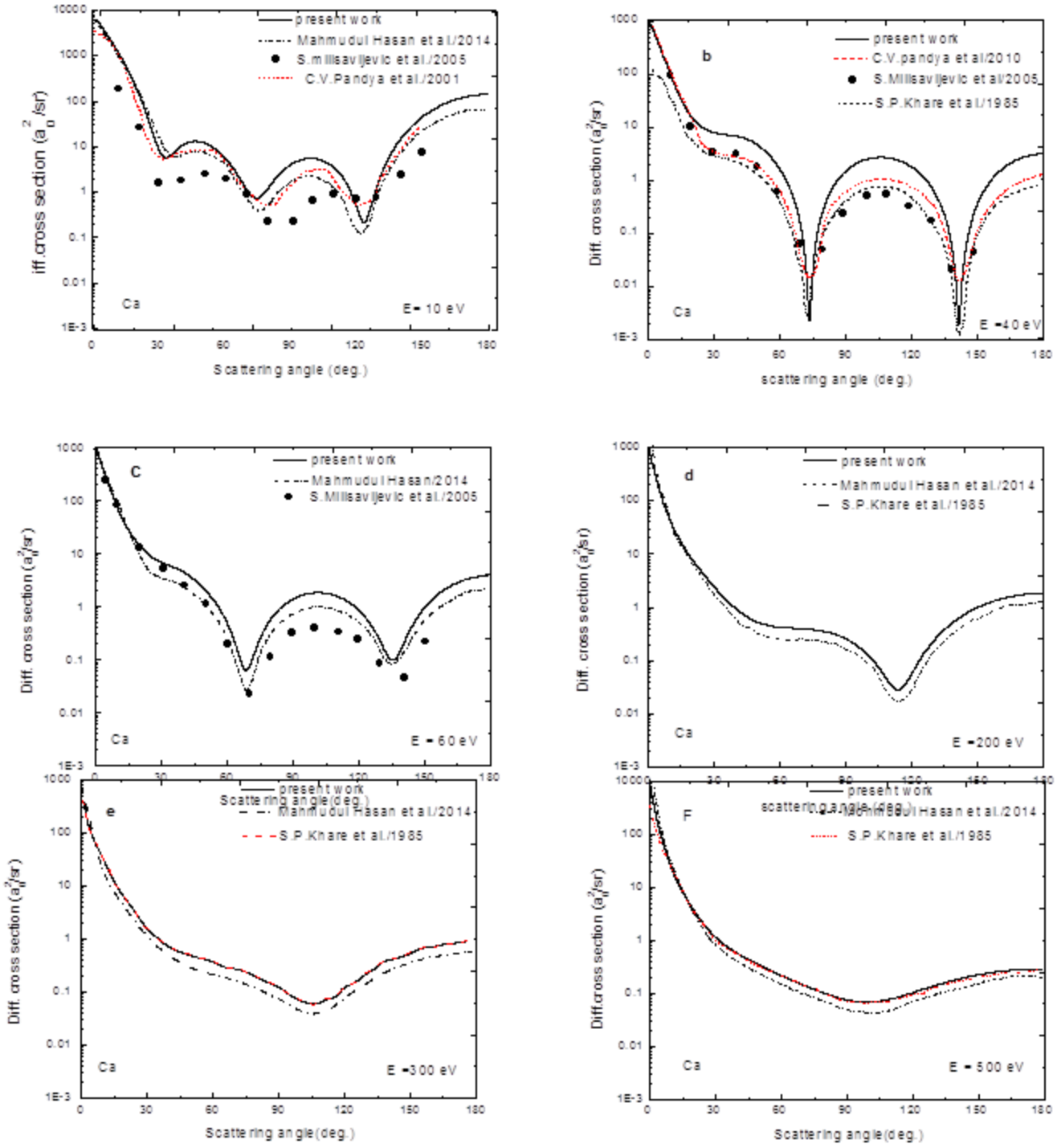


Figure (4): Differential cross-sections (a02/sr) for the Scattering of electrons from Ca- atoms for an incident electron energy (a)10 eV ,(b)40 eV,(c) 60 eV, (d) 200 eV,(e) 300eV, and (f)500 eV.

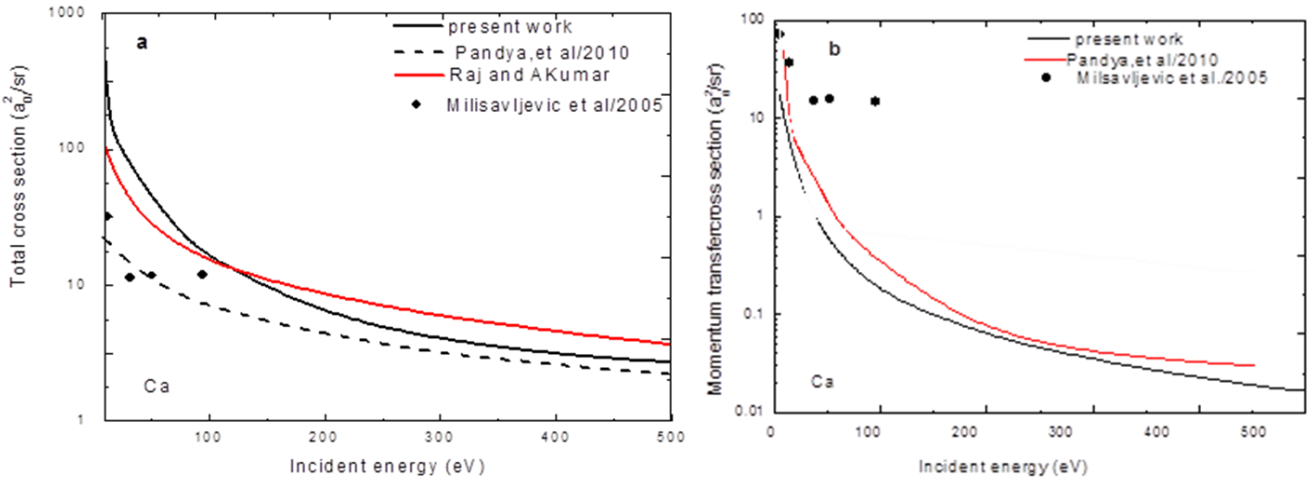


Figure (5): Total Cross – Sections(a20) for the Scattering of electrons from Ca- atoms in the impact electron energy range (1- 500) eV.

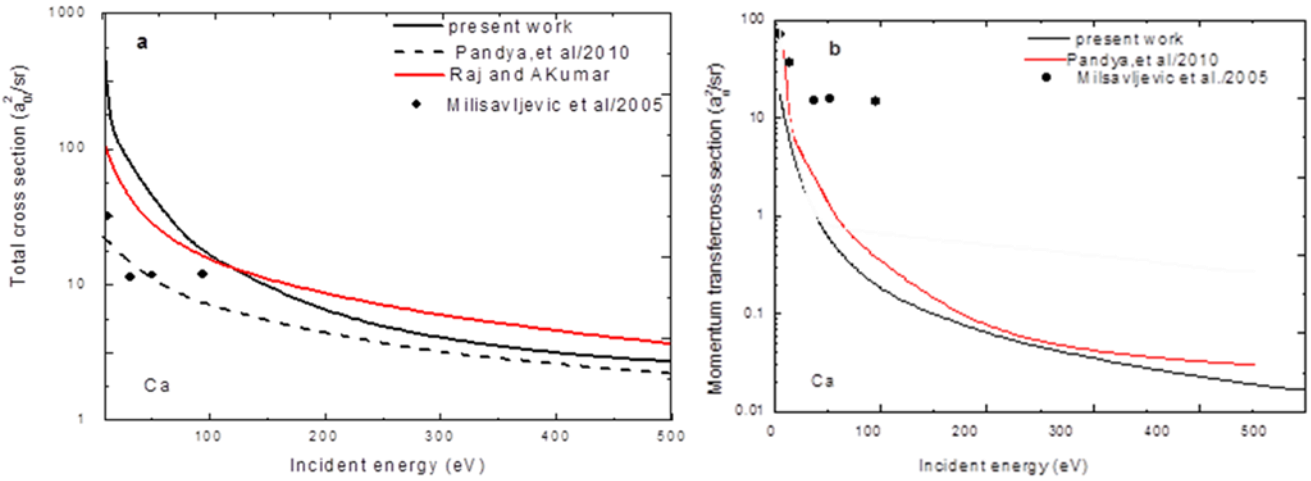
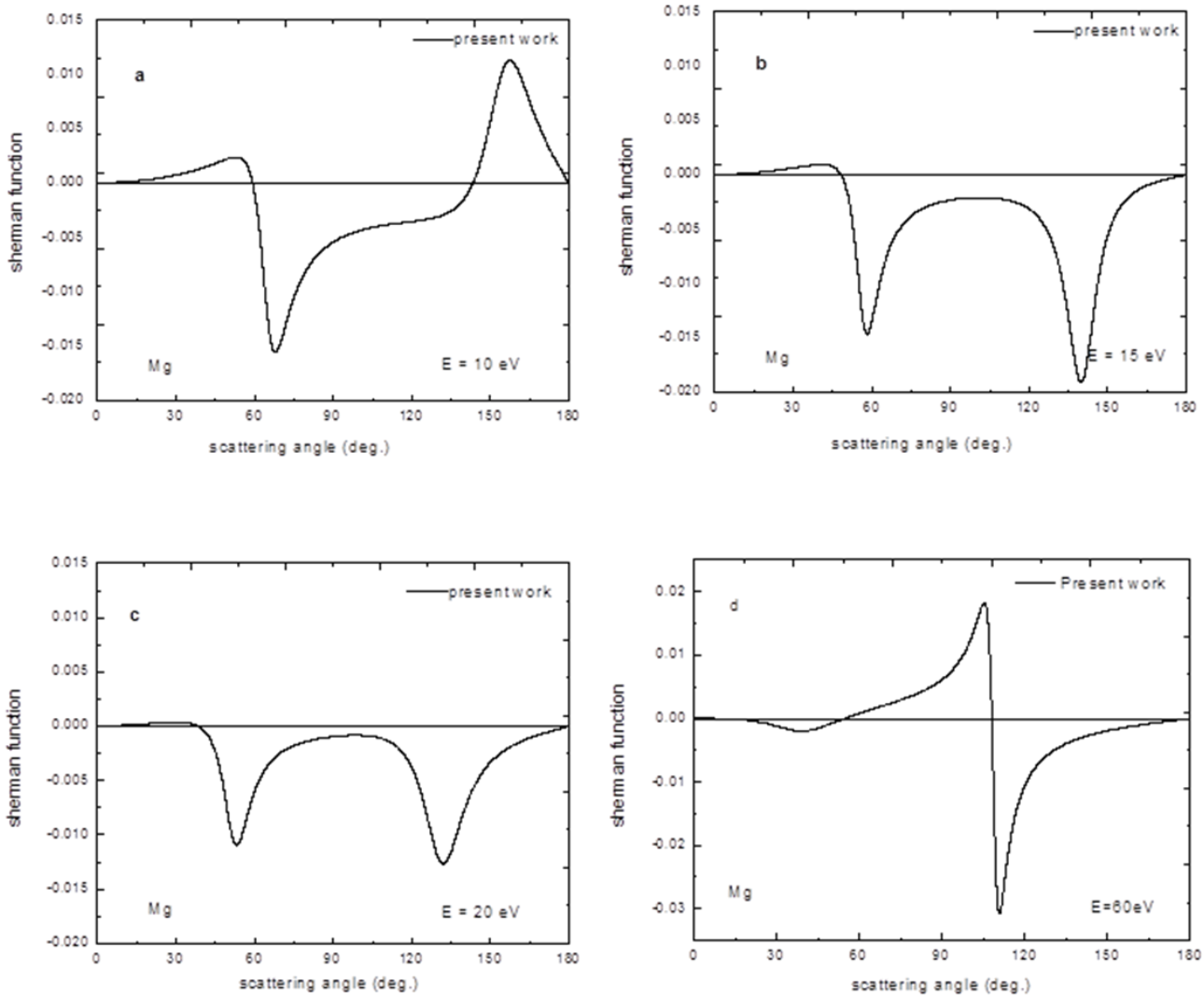
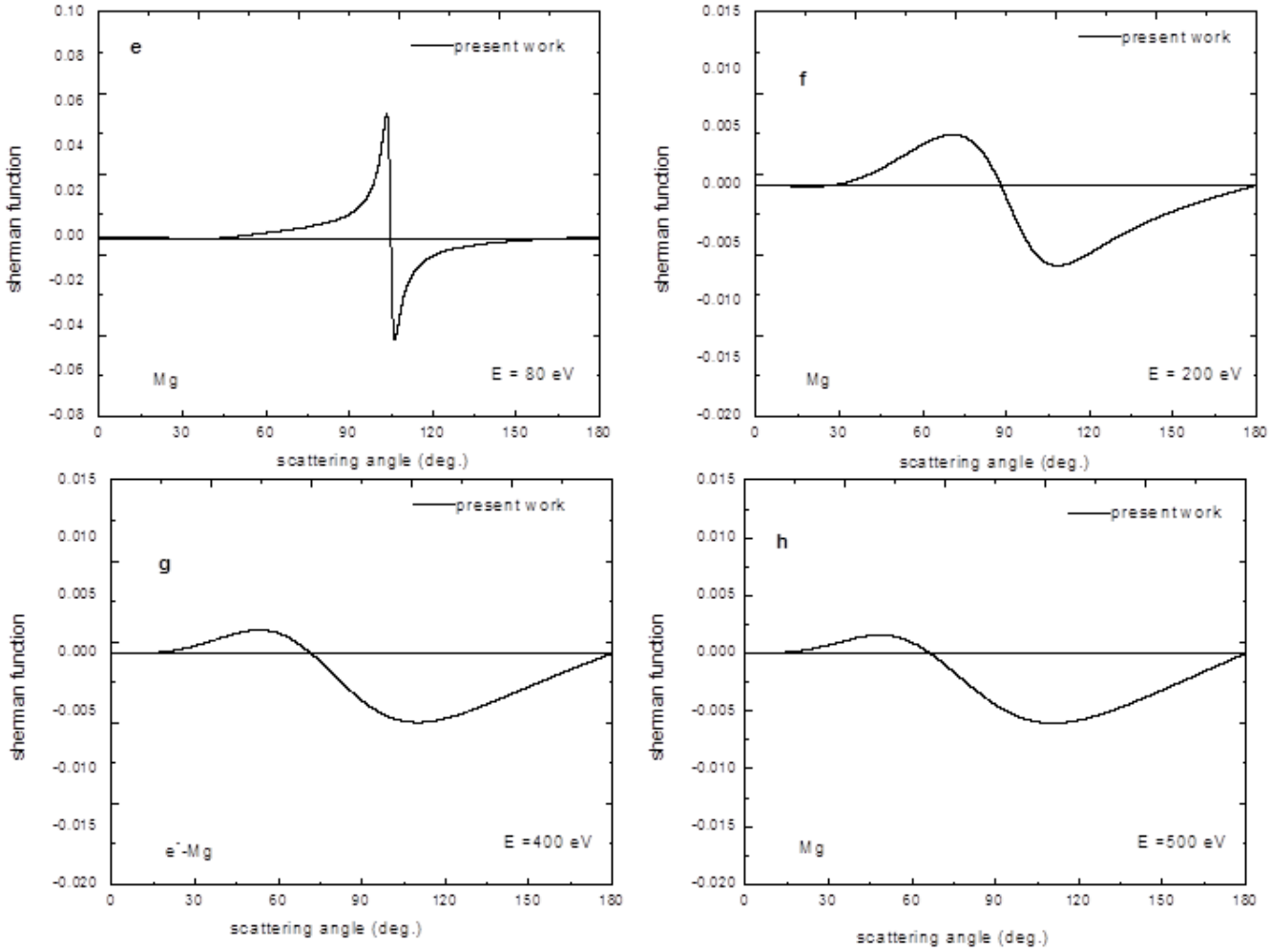


Figure (6): Momentum transfer cross-sections (a02) for the scattering of electrons Ca-atoms

In the incident electron energy range (1- 500) eV.



Figure(7):The variation of spin polarization parameter (S) with scattering angle at incident energies(a)10 eV,(b)15 eV (c)20 eV (d)60 eV.



Figure(7):The variation of spin polarization parameter (S) with scattering angle at incident energies(e)80 eV,(f) 200 eV (g) 400 eV (h) 500 eV.

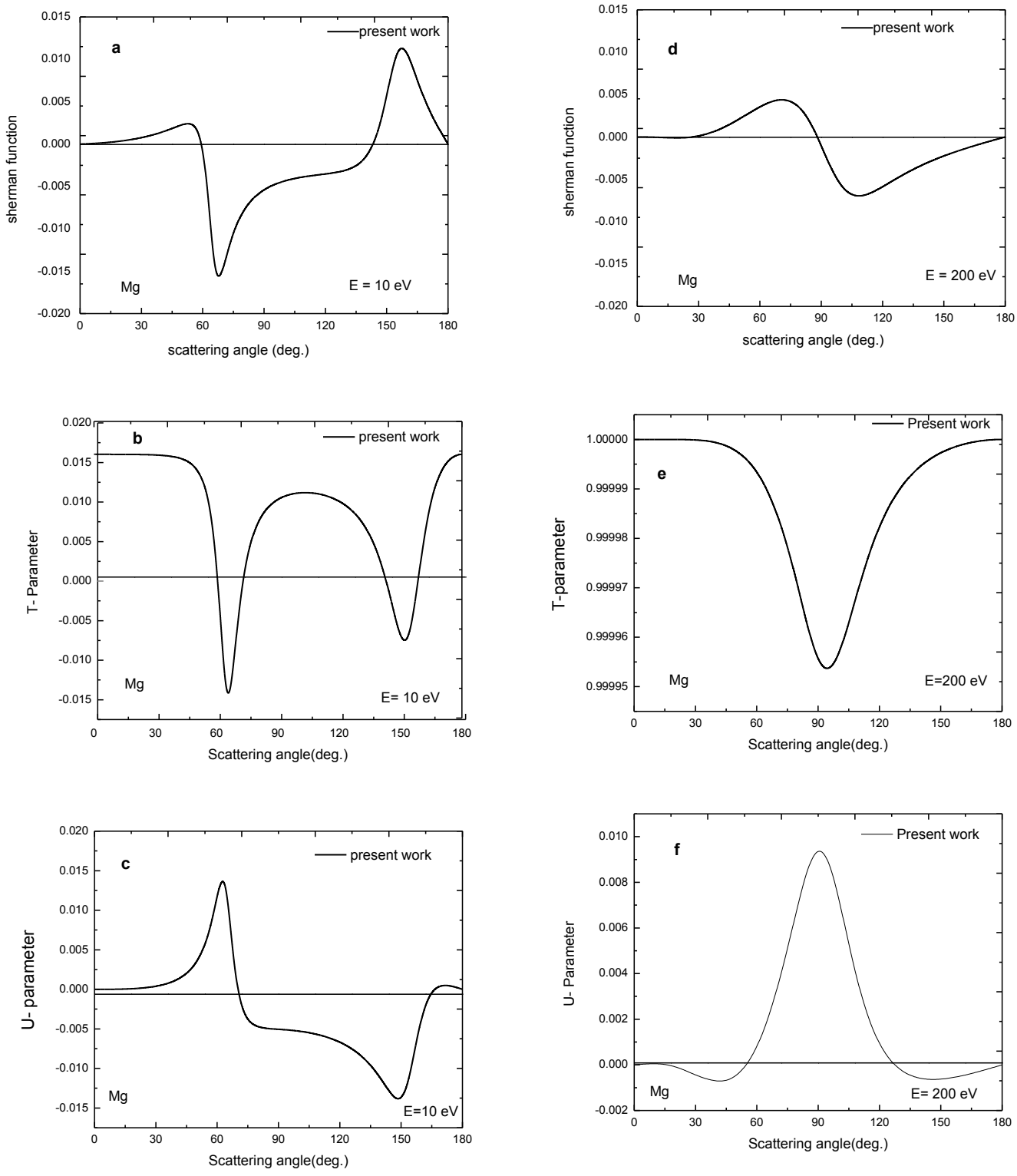


Figure (8): Spin polarization parameters S ,T, and U at 10eV for scattering of (a ,b , c) and at 200 eV of (d ,e ,f) for Mg – atoms.

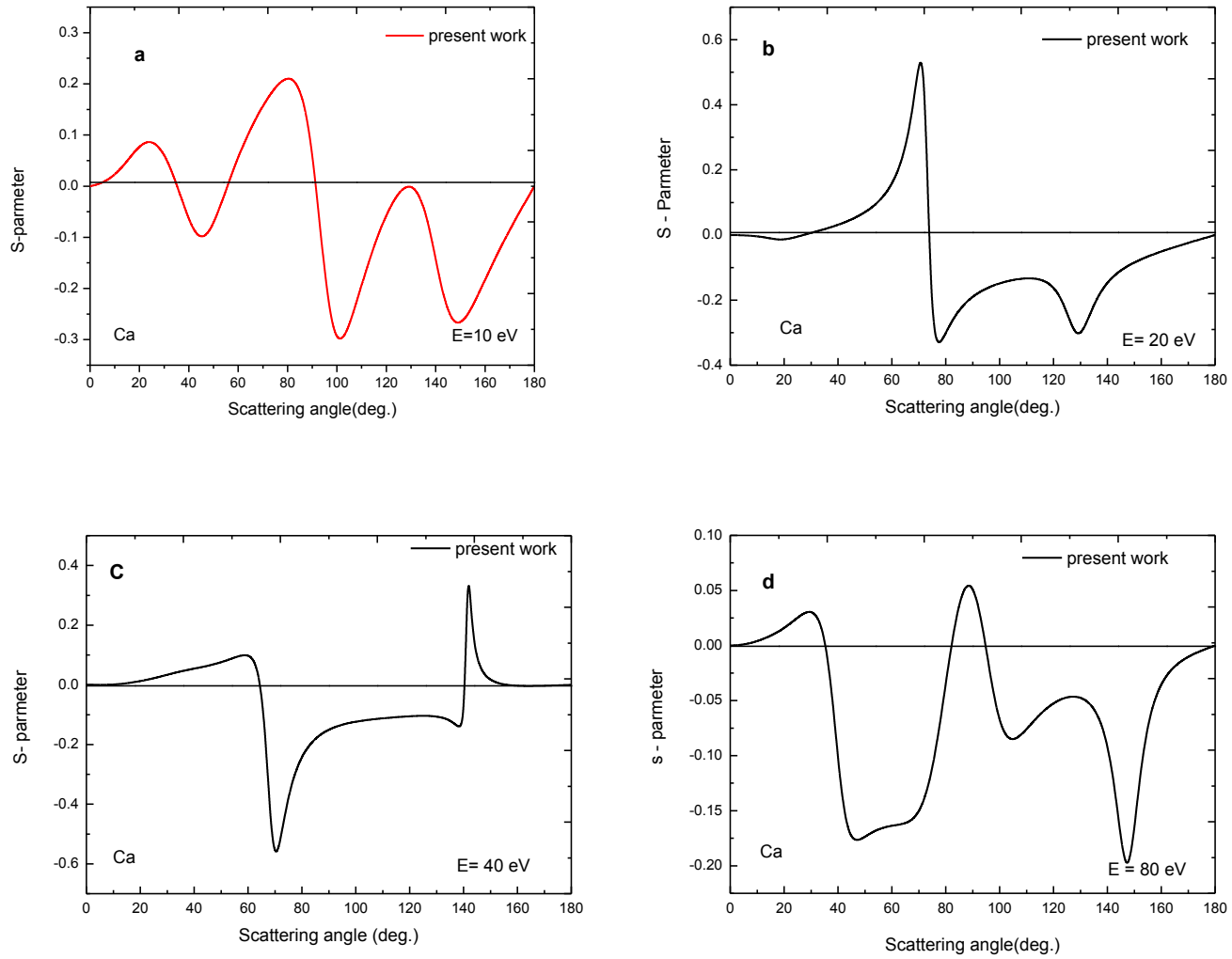


Figure (9):The variation of spin polarization parameter(S) with scattering angle at incident energies(a)10 eV ,(b)20 eV, (c) 40 ev, and (d) 80 eV.

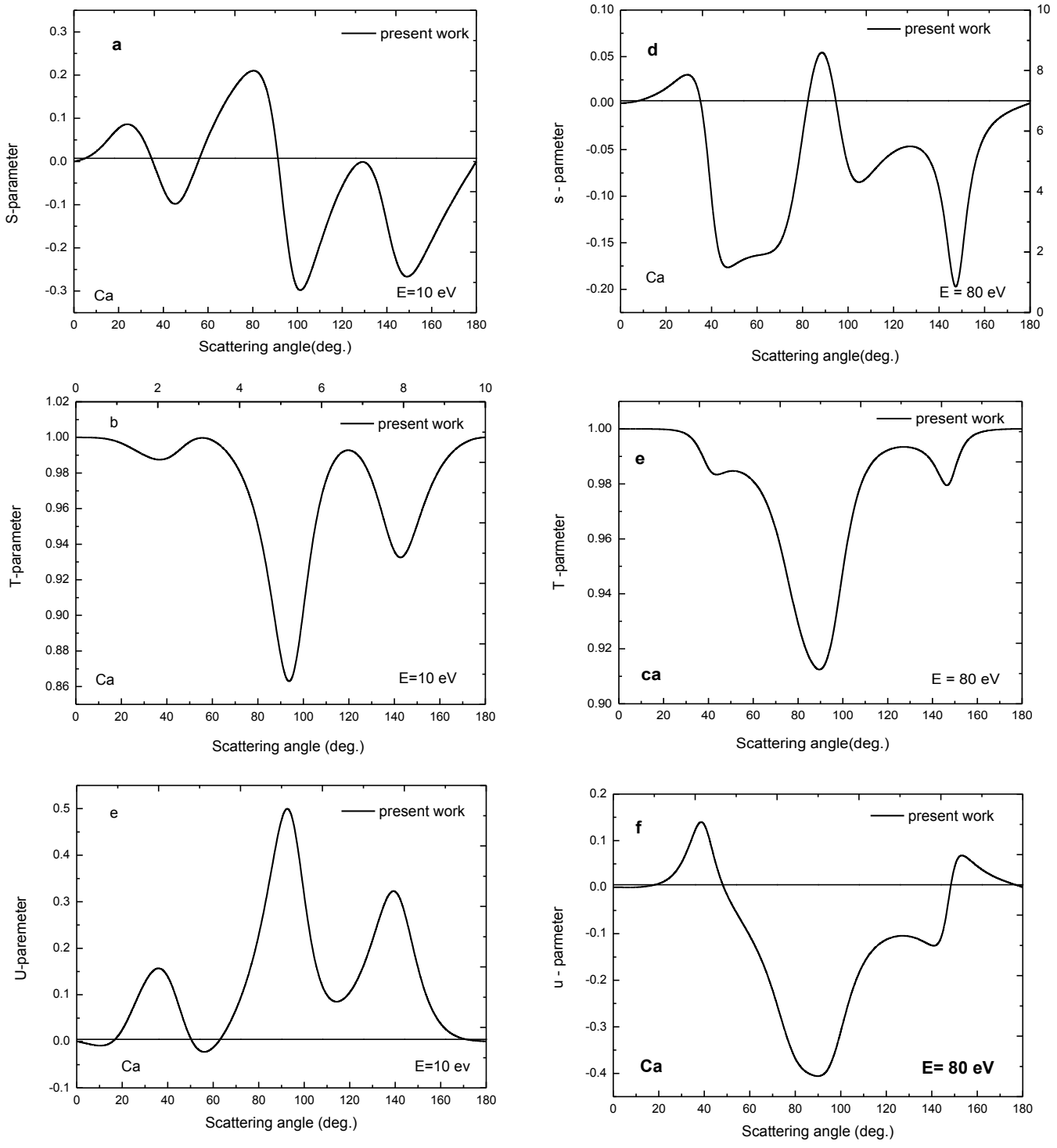


Figure (10): Spin polarization parameters S ,T, and U at 10eV for scattering of (a ,b , c) and at 80 eV of (d ,e ,f) for Ca – atoms.

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