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Research Article

Differential and Total Cross-Sections for Elastic Scattering of Electrons by Cadmium Atoms

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Abstract
The differential cross sections (DCS's), and total cross sections (TCS's) for the elastic scattering of electrons from Cadmium atoms in the energy range of (6.4-300) eV are calculated using the relativistic Dirac equations within partial wave analysis by using an optical-model potential. The optical potential used in this paper consist of many interactions. The electrostatic interaction is determined from the Dirac-Hartree-Fock self-consistent atomic electron density, the exchange interaction is described by means of the local-approximation of Furness and McCarthy. The correlation-polarization potential is obtained by combining the correlation potential of perdew and wang derived from the local density approximation with a long-range polarization interaction, which is represented by means of a Buckingham potential with an empirical energy dependent cutoff parameter. This model shows , a good agreement with the experimental measurements and the available theoretical results of other investigators.

1. Introduction

The relativistic interaction plays an important role in understanding the theoretical studies of different scattering functions such as cross sections in the scattering of electrons from heavy atomic targets [1] . A few investigations have been made of electrons scattering from cadmium to obtain the scattering functions of this comparatively heavy atom (Z=48) [2].In the present work , the Scattering potential includes the static [3] , exchange [4] and correlation-polarization [5] potentials .The effect of exchange potential is important for electron impact scattering .The correlation-polarization potential is a combination of the short range of Perdew-Wang correlation [6] and long range polarization of Buckingham model [7] ,the polarization is an important effect in low energy electron scattering when an electron slowly reach the atom ,the bound electrons are influenced by the electric field of the electron charge ,and an adiabatic redistribution of bound electronic density occurs, resulting in an dipole moment on the target atom [8] .

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In the present work, the calculation is performed on the Cadmium atomic target using the relativistic approach, by solving the Dirac equation to describe the scattering system in order to calculate the various cross sections according to scattering at low impact energies from 6.4 eV up to 300 eV. This relativistic treatment of electron scattering enables us to get all necessary information about collision process.

In sec. 2.1 ,the theory used in this work will be introduced , in which the partial wave analysis computational method used in present work , the calculated differential ,and total cross-sections will be described ,While in sec.2.2 ,the interaction between an electron and a target atom will be introduced. sec.3, deals with the results and discussion obtained from the calculated results , the conclusions are given in sec.4 .

2. Theory

2.1. Partıal Wave Analysis

The Dirac equation for a projectile of rest mass m_o in a central field $V(r)$ at a velocity v is given by [9] :

$$[c\boldsymbol{\alpha}.\boldsymbol{p} + \boldsymbol{\beta} m_o c^2 + V(r)]\Psi = E\,\Psi \qquad \ldots (1)$$

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 . And $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are the usual 4×4 Dirac matrices. The solutions of the Dirac equation has the form [7] :

$$\Psi_{E\kappa m}(r) = \frac{1}{r}\begin{pmatrix} P_{E\kappa}(r)\Omega_{\kappa,m}(\widehat{r}) \\ iQ_{E\kappa}(r)\Omega_{-\kappa,m}(\widehat{r}) \end{pmatrix} \qquad \ldots(2)$$

Where $\Omega_{k,m}(\widehat{r})$ are the spherical spinors ,while $P_{E\kappa}(r)$ and $Q_{E\kappa}(r)$ are the radial functions which satisfy the Dirac equations :

$$\frac{dP_{E\kappa}(r)}{dr} = -\frac{\kappa}{r}P_{E\kappa}(r) + \frac{E - V(r) + 2m_o c^2}{\hbar c}Q_{E\kappa}(r) \qquad \ldots(3)$$

And

$$\frac{dQ_{E\kappa}(r)}{dr} = -\frac{E - V(r)}{\hbar c}P_{E\kappa}(r) + \frac{\kappa}{r}Q_{E\kappa}(r) \qquad \ldots(4)$$

The relativistic quantum number κ is defined as $\kappa = (l - j)(2j + 1)$, where j and l are the total and orbital angular momentum quantum numbers determined by the value of κ , $j = |\kappa| - \frac{1}{2}$, $l = j + \frac{\kappa}{2|\kappa|}$. By normalization the spherical waves, the large-component radial function $P_{Ek}(r)$ oscillates asymptotically with unit amplitude. Therefore, for finite-range fields and $r \to \infty$, the proper solution of the radial function $P_{Ek}(r)$ behaves asymptotically as :

$$P_{Ek}(r) \cong \sin\left(kr - l\frac{\pi}{2} + \delta_k\right) \qquad \ldots(5)$$

Where $P_{Ek}(r)$ expressed in terms of the complex phase-shift δ_k . The relativistic wave number of the electron k , is related to the momentum p , and kinetic energy E_i , by $p = \hbar k$, and $k^2\hbar^2c^2 = {E_i}^2 - m_o^2c^4$, here, c is the velocity of light in

vacuum. In the present calculation, equations (2) and (3) satisfying the asymptotic condition (4) are solved numerically using RADIAL package [10] to extract the phase-shifts $\boldsymbol{\delta_k}$ and then to obtain the direct scattering amplitude $\boldsymbol{f(\theta)}$ and spin-flip amplitude $\boldsymbol{g(\theta)}$ arising from the in-built spin-orbit interaction in the Dirac equation. These amplitudes are given by the relations [11,12] :

$$\boldsymbol{f(\theta) = \frac{1}{2iK}\sum_{l=0}^{\infty}\{(l+1)[\exp(2i\delta_{k=-l-1}) - 1] + l[\exp(2i\,\delta_{k=l}) - 1]\}P_l(\cos\theta)} \quad \ldots(6)$$

And

$$\boldsymbol{g(\theta) = \frac{1}{2iK}\sum_{l=0}^{\infty}[\exp(2i\delta_{k=l}) - \exp(2i\delta_{k=-l-1})]P_l^1(\cos\theta)} \quad \ldots(7)$$

Where, $\boldsymbol{\theta}$ is the scattering angle, $\boldsymbol{P_l(\cos\theta)}$ and $\boldsymbol{P_l^1(\cos\theta)}$ are Legendre polynomials and associated Legendre functions, respectively. In this work , we have used ELSEPA code [7] ,to calculates phase-shift in increasing order of $\boldsymbol{l}$ up to a maximum value $\boldsymbol{l_{max}}$,for which the magnitude of the phase-shift $\boldsymbol{(\delta_k)}$ becomes smaller than 10^{-9}. So, partial-wave expressions for $\boldsymbol{f(\theta)}$ and $\boldsymbol{g(\theta)}$ converge to accuracy of more than six decimal places for all angles. The elastic differential cross section for the scattering of the unpolarized incident electron beam is given by [11]:

$$\boldsymbol{\frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2} \quad \ldots(8)$$

also , the total elastic cross section,

$$\boldsymbol{\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{\pi}(|f(\theta)|^2 + |g(\theta)|^2)2\pi \sin\theta d\theta} \quad \ldots(9)$$

2.2 Interaction Potential

The total interaction between an electron and a target atom is described by an effective potential $\boldsymbol{V(r)}$ which is chosen to be a sum of three terms, the static $\boldsymbol{V_{st}(r)}$,exchange $\boldsymbol{V_{ex}(r)}$, and the correlation-polarization $\boldsymbol{V_{cpol}(r)}$, potentials. These terms are functions of the electronic density of the target and approximately account for the dynamics of the collision and given by the following relation :

$$\boldsymbol{V(r) = V_{st}(r) + V_{ex}(r) + V_{cor}(r) + V_{pol}(r)} \quad \ldots(10)$$

The electrostatic interaction energy between the projectile and the target atom is obtained by [7]:

$$\boldsymbol{V_{st}(r) = \mathbb{Z}_o e\varphi(r) = \mathbb{Z}_o e[\varphi_n(r) + \varphi_e(r)]} \quad \ldots(11)$$

Where $\boldsymbol{\mathbb{Z}_o e}$ is the charge of the projectile ($\boldsymbol{\mathbb{Z}_o = -1}$) for electrons and $\boldsymbol{\varphi(r)}$ is the electrostatic potential of the target atom which is consist of the sum of contributions from the nucleus and the electron cloud, $\boldsymbol{\varphi_n(r)}$ and $\boldsymbol{\varphi_e(r)}$, generated from the electronic and nuclear charge distribution, respectively. Fermi nuclear charge distribution $\boldsymbol{\rho_n(r)}$ given by Hahn et al.[13] are adopted in present work to generate $\boldsymbol{\varphi_n(r)}$ .On the other hand , it has used the most accurate electron densities $\boldsymbol{\rho_e(r)}$ available for free atoms which are obtained from self-consistent relativistic Dirac–Fock (DF) calculations [14] to generate $\boldsymbol{\varphi_e(r)}$. The same density $\boldsymbol{\rho_e(r)}$ is used to obtain the electron exchange potential. In the present work, the exchange potential model of Furness and McCarthy[4] which is local

approximation to the exchange interaction is used to perform the calculations and is given by :

$$\boldsymbol{V_{ex}(r) = \frac{1}{2}\left(E_i - V_{st}(r)\right) - \frac{1}{2}\left[(E_i - V_{st}(r))^2 + 4\pi a_o e^4 \rho_e(r)\right]^{1/2}} \quad \ldots(12)$$

Where $\boldsymbol{E_i}$ is the kinetic energy of the projectile, $\boldsymbol{a_o}$ is the first Bohr radius. For the correlation-polarization potential $\boldsymbol{V_{cpol}(r)}$,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 $\boldsymbol{V_{cor}(r)}$ and the long-range $\boldsymbol{V_{pol}(r)}$ parts and are given by [9] :

$$\boldsymbol{V_{cpol}(r) = \begin{cases} V_{cor} & if \quad r < r_c \\ V_{pol} & if \quad r \geq r_c \end{cases}} \quad \ldots(13)$$

Here, $\boldsymbol{r_c}$ is the point where the two forms cross each other for the first time. The short-range form $\boldsymbol{V_{cor}(r)}$ for electron scattering from atoms is based on an accurate analytic representation of the uniform electron-gas correlation energy as a function of density parameter $\boldsymbol{r_s}$, and relative spin polarization $\boldsymbol{\zeta(r)}$,the dependent parameters on $\boldsymbol{\zeta(r)}$ are calculated in the low and high density limits, on the other hand, the electron-electron correlation must be taken into account ,where the electrons of the atom are resisted by forming a "Coulomb hole" Handicap the incident electron when it penetrates through the charge distribution of the atom [15] .So, the electron-electron correlation is effective .In the present work, we adopted the parameterization of the correlation potential given by Perdew and Wang [6] , this potential for $\boldsymbol{r_s < 1}$ and $\boldsymbol{\zeta(r) = 0}$, high density limit , given by:

$$V_{cor}(r) = 0.031091 \ln r_s - 0.0570076 + 0.0044260\, r_s \ln r_s - 0.0091666 r_s \quad \ldots(14)$$

While for $\boldsymbol{r_s \geq 1}$ and $\boldsymbol{\zeta(r) = 0}$, low density , the form is :

$$\boldsymbol{V_{cor}(r) = -0.578\, r_s^{-1} + 2.1612\, r_s} \quad \ldots(15)$$

Where ,

$$\boldsymbol{r_s = \left(\frac{3}{4\pi\rho_e(r)}\right)^{1/3}} \quad \ldots(16)$$

$$\boldsymbol{\zeta(r) = \frac{\rho_{e\uparrow} - \rho_{e\downarrow}}{\rho_{e\uparrow} + \rho_{e\downarrow}}} \quad \ldots(17)$$

Where , $\boldsymbol{\rho_{e\uparrow}}$ and $\boldsymbol{\rho_{e\downarrow}}$ represent the spin density of electrons , hence , $\boldsymbol{\zeta(r) = 0}$ for Cadmium . Slow projectiles cause the polarization of the charge distribution of the target atom and, So, the induced dipole moment acts back on the projectile. When the projectile is far from the atom, the polarization potential energy can be approximated by means of the Buckingham potential [16] :

$$\boldsymbol{V_{pol} = -\frac{\alpha_d e^2}{2(r^2 + d^2)^2}} \quad \ldots(18)$$

where, $\boldsymbol{\alpha_d}$ is the atomic polarizability of the target atom. For Cadmium atom it is taken to be experimental value equal to $\boldsymbol{\alpha_d = 48.636\, a_o^3}$ [17] . And d is a phenomenological cutoff parameter, that serves to prevent the polarization

potential from diverging at $\boldsymbol{r = 0}$. Following Salvat [16], we use the expression given by Mittleman and Watson [18] for the cut-off parameter $\boldsymbol{d}$, as :

$$\boldsymbol{d^4 = \frac{1}{2}\alpha_d a_o Z^{-1/3} b_{pol}^2} \quad \text{...(19)}$$

Where , $\boldsymbol{a_o}$ is atomic unit assumed equal to one and $\boldsymbol{b_{pol}^2}$ is an adjustable energy-dependent parameter where it is given by [18] :

$$\boldsymbol{b_{pol}^2 = (E_i - 50\ eV)/(16\ eV)} \quad \text{...(20)}$$

So ,in this work the assuming is that the Buckingham polarization potential, is given by equations (18)-(20).While, the global correlation–polarization potential is determined by combining the Buckingham potential, equations (18)-(20), with the local density approximation correlation potential given by equations (14) - (17) according to equation (13).

3.Results and Discussion

In this work, we have calculated the differential cross sections, and total cross sections for elastic scattering of electrons from Cadmium atoms at various impact energies between (6.4-300) eV. The results are performed relativistically by using an interaction potential in Dirac equation. We compared our results with the available theoretical values of Haque et.al.[19] and Nahar [2] and experimental measurements of Marinkovic et.al.[20]. The results of differential cross sections are shown in figures (1) ,(2) and (3). Where our values of differential cross sections, agree reasonably well with the available theoretical values of Nahar [2] , Haque et.al.[19] and experimental measurements of Marinkovic et.al.[20] especially at at high energies ,as shown in figures (2) and (3) . There is a slightly differences between our results and the results of others occurs at low impact energies ≤ 20 eV as shown in figures (1)a -(1)c , because of the interaction potentials as well as the relativistic correction 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 others. On the other hands, the effects of the polarization, correlation and the exchange become negligible at high energies, only the static potential dominate, so at high energies the differences become neglected.

Figure 1. Differential cross sections for scattering from Cadmium atoms at electron energies (a) 6.4 eV,(b)10 eV ,(c) 20 eV ,(d) 40 eV .

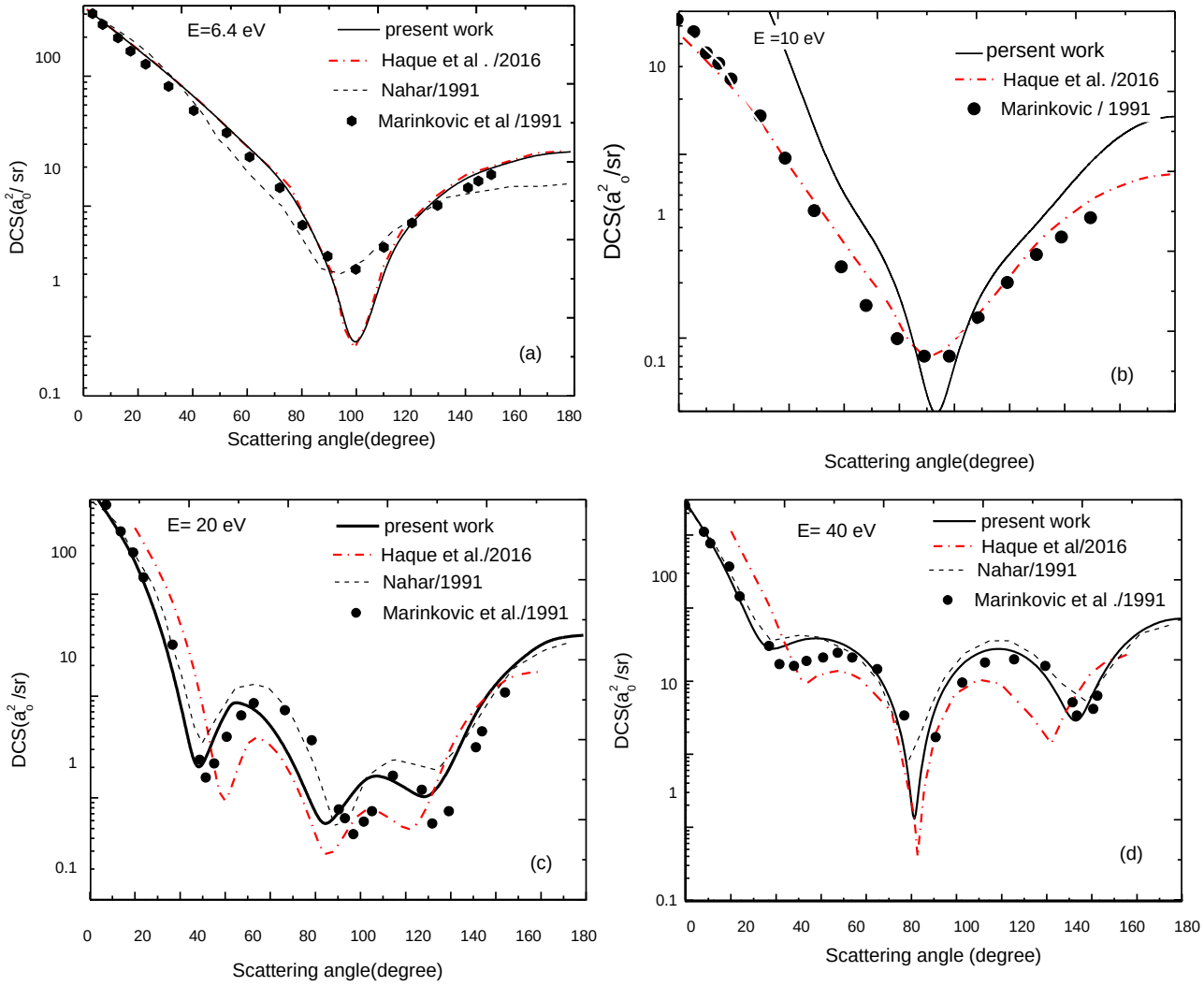


Figure 2. same as FIGURE 1 but for electron energies (e) 60 eV,(f) 75 eV , (g) 85 eV ,(h) 100 eV.

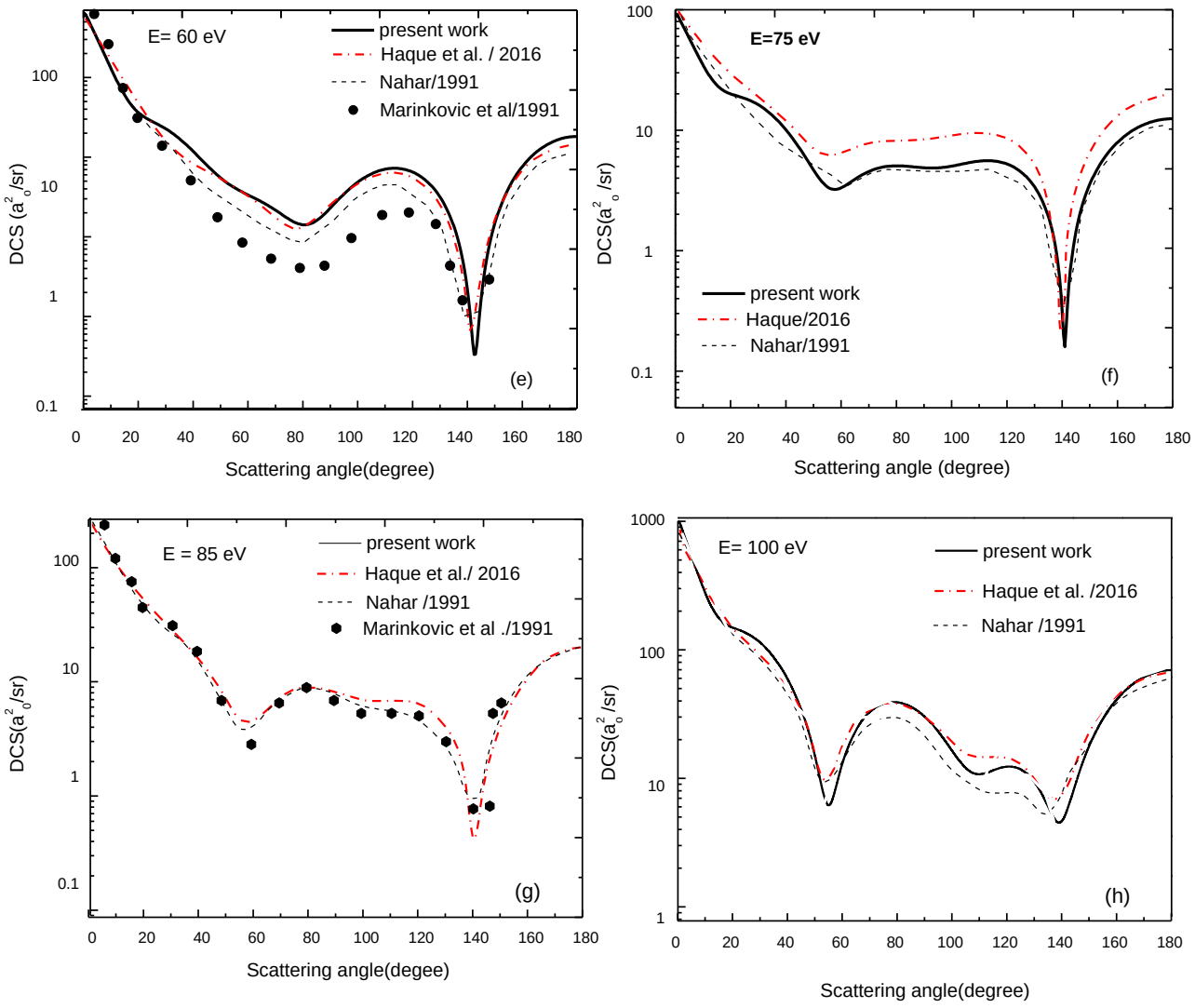


FIGURE (4). Illustrates the total cross sections for Cadmium atoms .Our results compared with the theoretical data of Haque et al.[19] and Nahar [2],but there is no experimental measurements. From figure (4), it can be observed that total cross sections have the highest values at low energies and reasonably agree well with the result of Haque et al.[19] and slightly agree with curve of Nahar [2] , because of the central potential used, where the static potential is completely determined by the adopted nuclear and electronic charge density model which is differ from that used by Nahar [2]. Also, the correlation –polarization potential models considered in this work combine empirical information with the local density approximation ,while Nahar [2] has been used only polarization without correlation potential for the short and long range limit.

Figure 3. same as FIGURE 1, but for electron energies (i) 200 eV,(j) 300 eV.

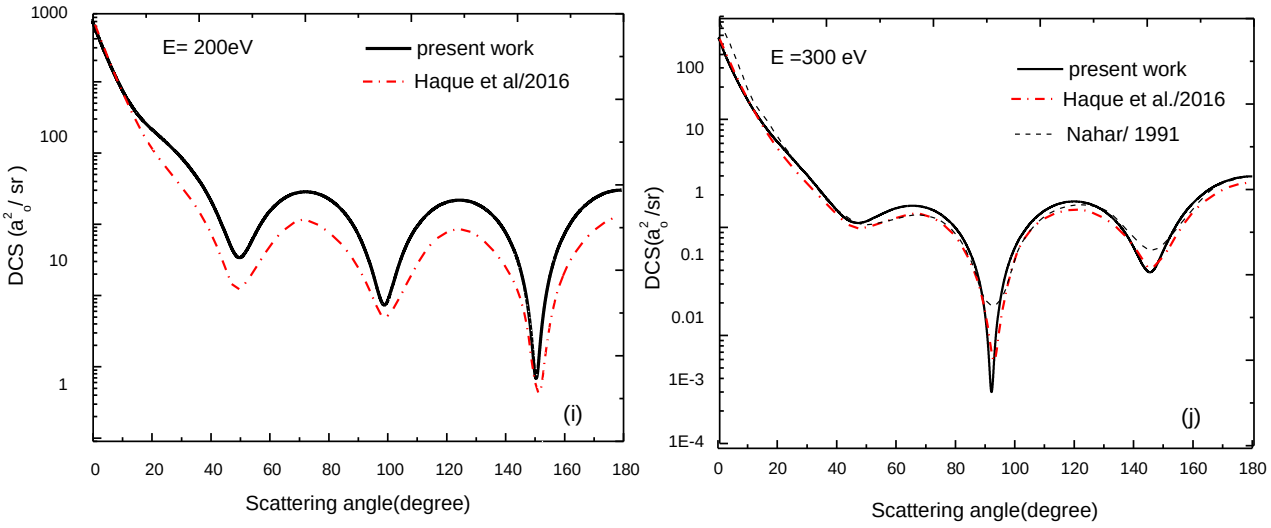
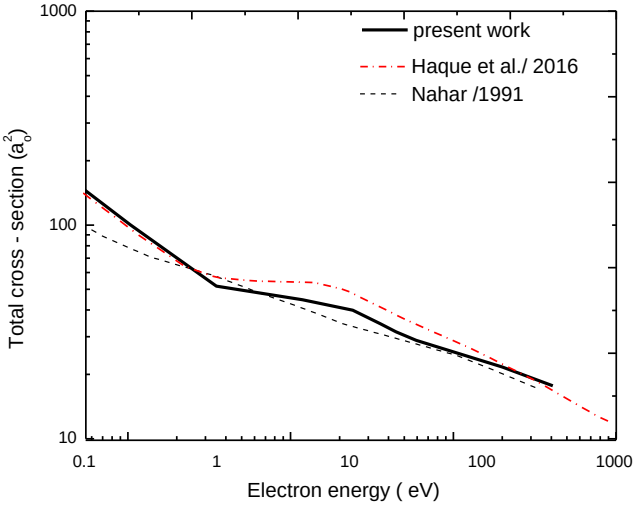


Figure 4. Total cross sections (a_o^2) for scattering by Cadmium atoms .



4. Conclusions

The elastic scattering of electrons from Cadmium atom has been treated relativistically by solving the Dirac equation numerically for the model potential representing the projectile-target interaction which is consists of static, exchange and correlation-polarization terms. These terms are important for Cadmium 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 effects in the Dirac equation, becomes more important at low energies. Generally, the scattering functions obtained in this work show good agreement with the results of other investigators, but there is a slightly some

differences between our results for differential, and total cross-sections with results of others , because of the absorption component of the optical potential where not included it in whole scattering potential .

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