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Investigation of Scattering Cross Sections for Electrons Colliding with Silver Atom

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***Abstract*—A relativistic approach is employed to compute the elastic differential cross sections for the scattering of electrons from silver (Ag) atom in low energy region i.e. at 10, 20 and 40 eV. The projectile–target interaction is composed of three local and real terms i.e. static, exchange and polarization potentials. The total optical potential is then used in the solution of the Dirac equation for scattered electron. The present calculated angular distributions show a reasonably good agreement with the measured values compared to other calculations.**

***Index Terms*—Electron, scattering, cross sections.**

I. INTRODUCTION

SCATTERING of electrons with atoms provides useful information for understanding of their structures and reaction mechanism in terms of scattering cross sections. These cross sections are of particular relevance in the field of technology, astrophysics, plasma and biomedical sciences. For example, in astrophysics, scattering cross sections are required for the spectrum analysis, chemical composition determination of various astrophysical objects and also for its abundance analysis [1-3]. Similarly, these are also needed in the calculation of plasma parameters [4, 5] used in the plasma diagnostic and modeling technique. In this paper we have considered electron interaction with silver atom at low energy. The reason for choosing silver as a target atom is that it has the highest thermal and electrical conductivity with the number of applications. Further, silver is an integral part of ornamental designing in Indian traditions. In recent years several groups [6-10] worked for determination of scattering cross sections of electrons with atoms. Tosic *et al.* [11] have performed both experimental measurements as well as theoretical calculations for differential cross sections of this system. They have measured the differential cross sections at electron impact energies of 10, 20, 40, 60, 80 and 100 eV based on crossed beam technique and have performed calculations using the parameter-free complex optical potential with the inclusion of spin-orbit interaction. It is noticed that their experimental and theoretical results differ considerably and therefore needs further investigations. Arnal *et al*. [12] have calculated and measured electron scattering cross sections for aluminum, copper, silver and gold samples at increased energies i.e. from 300 – 1200 keV. He developed a theory similar to that of Lenz using a modified form of the Wentzel potential. The influence of the spin in the elastic low-energy scattering from gaseous atoms has been investigated by Fink and Ingram [13]. They used relativistic Hartree–Fock–Slater scattering potential in solving the Dirac equation, but excluding the exchange of the incident electron with the atomic electrons and the polarization. The calculations of Salvat *et al*. [14] employed the CPC code of Yates [15] without using the polarization and the exchange potentials at energies greater than 100 eV. Further, he also used a method given by Bonham and Strand [16] to solve the Dirac equation using empirical potential. Jablonski *et al*. [17] analyzed differential cross sections (DCS) for six elements containing silver at the energies from 100 to 10,000 eV. These DCS have been derived from two potentials, i.e. Thomas–Fermi–Dirac (TFD) and Dirac–Hartree–Fock (DHF) potentials. The differential cross sections of electron-silver atom are calculated using the Eikonal approximation with the Lenz-Jensen potential by Abdu *et al*. [18] at energies 50, 60 and 70 eV. In this paper we have made an attempt to calculate the elastic differential cross sections for silver atoms in this low energy region i.e. from 10 to 40 eV.

II. THEORETICAL METHODOLOGY

In the present study, motion of the projectile electron in a central field $V(r)$ is described by the Dirac equation given as:

$$[c\alpha.p + \beta m_0 c^2 + V(r)]\psi = E\psi \quad (1)$$

where $E = m_0\gamma c^2 = E_i + m_0c^2$ is the total energy of incident electron, $\gamma = (1 - v^2/c^2)^{-1/2}$ and E_i is the kinetic energy of the incident electron. α and β are the 4 x 4 Dirac matrices. The spin or ψ has four components and $\psi = (\psi_1, \psi_2, \psi_3, \psi_4)$,

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where (ψ_1, ψ_2) are the large components and (ψ_3, ψ_4) are the small components of ψ. For a central potential, the Dirac equation can be reduced to a set of two equations similar to the Schrodinger equations [19, 20]

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

where $g_l^{\pm}$ is related to the radial part $G_l^{\pm}$ of the large component of ψ by

$$G_l = \sqrt{\eta}\, g_l / r,$$

$$\eta = (E - V + m_0 c^2)/c\hbar \text{ and}$$

$$K^2 = (E^2 - m_0^2 c^4)/\hbar^2 c^2.$$

The effective Dirac potential terms $U_l^{\pm}(r)$ expressed in atomic units are given by

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

where α is the fine-structure constant (not to be confused with the Dirac matrix α). The single and double primes denote the first and second order derivatives with respect to *r*.

Here, the total interaction between an electron and the target atom is approximately represented by an effective potential which can be expanded in terms of symmetry-adapted function of the A_1 irreducible representation (totally symmetric)

$$V_{\text{eff}}(r) = \sum_{l,\,h} V_{l\,h}(r)\; X_{l\,h}^{A_1}(r) \tag{4}$$

Retaining only the first term (l = 0, h = 1) in the expansion of Eq. 4, the spherical potential is then written as the sum of three local and real terms, namely, the static (V_{st}), the exchange (V_{ex}) and the polarization (V_{pol}) parts, which approximately account for the dynamics of the collision process. All these potentials are functions of the electronic density of target atom. The static potential of the target atom is obtained by averaging over the motion of the target electrons and is given

$$V_s(r) = \frac{Zee_p}{r} - ee_p \sum_n \sum_l \sum_m N_{nlm} \int |\phi_{nlm}(\mathbf{r}')|^2 \frac{1}{|\mathbf{r} - \mathbf{r}'|}\, d\mathbf{r}', \tag{5}$$

where Z is the nuclear charge of the target atom. e_p is the projectile charge and N_{nlm} is the occupancy number of the orbit (n, l, m). The radial part $\varphi(r)$ of the spatial orbital

$$\varphi_{n\,l\,m}(r) = \varphi_{n\,l}(r) y_{l\,m}(\hat{\mathrm{r}})$$

is expanded in terms of Slater-type orbitals given in the tables of Clementi and Roetti [21] and Mclean and Mclean [22].

In the present calculations, the modified semi-classical exchange (MSCE) potential (V_{ex}) have been used, which is taken from Gianturco and Scialla [23].

$$V_{\text{ex}}^{\text{MSCE}}(r) = \frac{1}{2}\left\{E - V_{\text{st}}(r) + \frac{3}{10}\left[3\pi^2\rho(r)\right]^{2/3}\right\} - \frac{1}{2}\left\{\left[E - V_{\text{st}}(r) + \frac{3}{10}\left[3\pi^2\rho(r)\right]^{2/3}\right]^2 + 4\pi\rho(r)\right\}^{1/2} \tag{6}$$

The electronic density of the target atom is distorted by the impinging electron. Therefore the exchange potential by including polarization of the target atom wave function gets modified. This must be taken into account by replacing V_{st} by $V_{\text{D}} = V_{\text{st}} + V_{\text{pol}}$ in eq. (6).

The term polarization potential is based on the correlation energy of target atom. Here, we have used a parameter-free polarization potential (V_{pol}). It has two parts the short range [$V_{\text{SR}}(r)$] and the long range [$V_{\text{LR}}(r)$], and is given by

$$V_{\text{pol}}(r) = \begin{cases} V_{\text{SR}}(r), & r < r_c, \\ V_{\text{LR}}(r), & r \geq r_c \end{cases} \tag{7}$$

where, r_c is the point where two forms cross each other for the first time. For the silver atom it is given by r_c = 5.58 a_0 point. The short-range form for the electrons scattering with atomic systems based on the free-electron gas exchange potential

$$V_{\text{SR}}(r) = \begin{cases} 0.0622\ln r_S - 0.096 + 0.018 r_S \ln r_S - 0.02 r_S, & r_S \leq 0.7 \\ -0.1231 + 0.03796\ln r_S, & 0.7 < r_S \leq 10.0 \\ -0.876 r_S^{-1} + 2.65 r_S^{-3/2} - 2.8 r_S^{-2} - 0.8 r_S^{-5/2}, & 10.0 \leq r_S \end{cases} \tag{8}$$

where, $r_s = [3/4\pi\rho(r)]^{1/3}$ and $\rho(r)$ is the electron charge density of the target atom. The long-range form of the polarization potential is given by $V_{\text{LR}}(r) = -\alpha_0/2r^4$, where α_0 is the dipole polarizability of the target. For the present calculations, The value of α_0 is taken [24] as 42.51 a_0^3.

III. Results and Discussion

In this paper, we present elastic differential cross sections

(DCS) only at those energies where both experimental as well as other theoretical results were available. Therefore, in Figs. 1-3 DCS are displayed at energies 10, 20 and 40 eV respectively. Note that in the present fixed nuclei approximation, the DCS are divergent in the forward scattering. The experimental DCS of Tosic *et al.* [11] are available at all of these energies along with their theoretical calculations. At 10 eV [Fig. 1], our DCS results are in good agreement with the experimental measurements of Tosic *et al.* [11] in the entire angular region except at middle angles between 80° and 105° compared to their calculations. At middle angles a dip appears similar to the calculations of Tosic *et al.* [11], but its magnitude is less and is in better agreement with measurements.

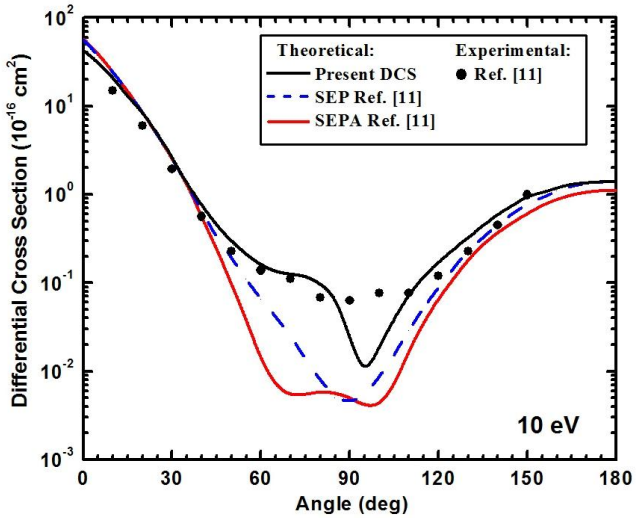

Fig. 1. Differential cross section for *e* – Ag system at 10 eV.

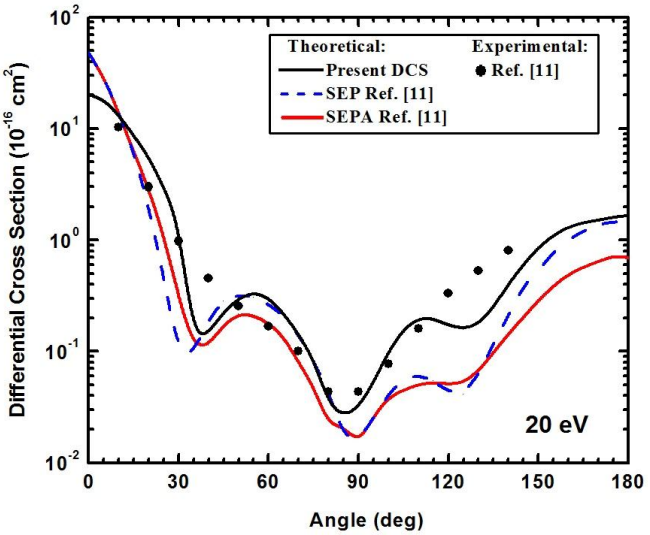

Fig. 2. Differential cross section for *e* – Ag system at 20 eV.

Moving to the next higher energies i.e. 20 and 40 eV [see Figs. 2 to 3], our results are in good agreement with the experimental measurements upto 110°. Beyond 110°, the present calculated DCS values show shallow dip and thereafter backward peaking slop compared to the measurements which are only available upto scattering angle 150°. The dip position agrees well with the two different calculations of Tosic *et al.* [11] but its magnitude is smaller and consequently our results are close to their experimental measurement.

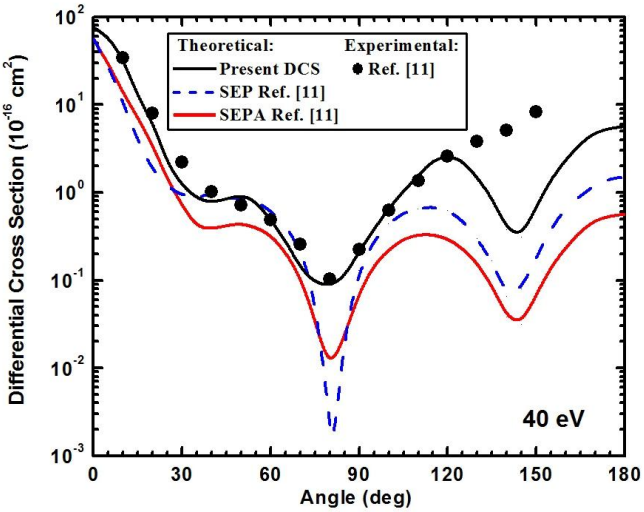

Fig. 3. Differential cross section for *e* – Ag system at 40 eV.

IV. Conclusion

We have presented results of our relativistic calculations of the elastic differential cross sections for electrons scattering from silver atom at energies 10, 20 and 40 eV. In these calculations, modified semi classical exchange potential is used to account for the effect of exchange of the scattering electron and target electron along with a parameter-free correlation polarization potential which accounts for the polarization of target charge cloud. The exchange, a parameter-free correlation polarization and static potentials are derived from the *ab initio* atomic charge density. The difference between present calculations and those of others can be said to be due to the different choices of both the the potential and the charge density which correctly simulate the required dynamical effects of scattering process. Further, the present results clearly show the importance of spin-orbit interaction which is included in a natural way through the Dirac equation in the present approach.

Finally, there is a need of experimental progress for *e* - Ag collisions for the assessment of present calculated results.

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