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Electron dichroism effects in the relativistic $(e, 2e)$ process for K-shell ionization of atoms

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Abstract. In this communication we present theoretical demonstration of electron dichroism in the relativistic $(e, 2e)$ process for K-shell ionization of atoms in non-coplanar asymmetric geometry. The theoretical formalism has been developed in plane wave Born approximation and in this approximation the triple differential cross-section (TDCS) has been expressed as a product of kinematical factors and atomic structure functions. The longitudinal spin asymmetry in the relativistic $(e, 2e)$ process on K-shell of atoms has been shown to depend on the interference between the transition charge and component of the transition current in the direction perpendicular to the scattering plane. Further, the longitudinal spin asymmetry has been shown to depend on incident electron energy, atomic number of the target, azimuthal angle of the ejected electron and scattered electron angle.

Keywords. Dichroism; chiral effect; longitudinal spin asymmetry; relativistic $(e, 2e)$ process.

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1. Introduction

The investigation of chiral and handedness effects, i.e. dichroism, in different collision problems $(\gamma, 2e), (e, 2e)$, positronium formation etc. with the atomic and molecular targets, holds a particular fascination and is of great importance in understanding the dynamics of the processes. The photoemission process from linear molecules either absorbed on the surfaces [1] or fixed in space [2] show the chiral effects. In this case the quantal axis of the molecule, the direction of the incident radiation and the momentum of the photoelectron form a right-handed reference frame. The same situation occurs in double photoionization, wherein the direction of the incident photon and the momenta of the two photoelectrons form a chiral system. Thus it is not surprising to observe chiral effects in highly symmetric systems, such as the ground state of helium, provided indistinguishability of the electrons is taken into account. To perform an experiment of this kind a circularly polarized light is needed and the two final electrons must be asymmetric either in energy or in flight direction. The circular dichroism in the atom was first predicted by Berakdar and Klar [3] and measured in terms of triple differential cross-section (TDCS). The experimental evidence for such an effect in He atom was given by Viefhaus *et al* [4] by using 93.5 eV photons. They also predicted the necessary conditions to observe a non-vanishing dichroism and the conditions are: (i) the two electrons unevenly share the excess energy and (ii) the direction of the incident radiation and two ejected electrons are not lying in one plane. The circular dichroism in $(\gamma, 2e)$ process on atom led to a number of experiments [5–7] designed to look for asymmetries in the interaction between the polarized electron/positron and chiral targets. Farago [8] was the first to propose that the collision between the longitudinally polarized electrons and chiral molecules will have new spin-dependent phenomenon in analogy with the optical activity and optical circular dichroism. In electron dichroism the attenuation of a beam of longitudinally polarized electrons depends on whether the polarization is parallel or anti-parallel to the beam direction and on whether the molecules are right- or left-handed. Blum and Thompson [9], Blum [10] and Thompson and Kinnin [11] have done extensive theoretical investigations of the electron dichroism. They have shown that the target chirality can be either due to the structure of the molecule or due to the geometry of the experiment.

Thompson and Blum [12] have demonstrated the chiral effects in the ionization of the oriented HCl molecule by low-energy longitudinally polarized electrons. They have computed the asymmetry in the ionization between parallel and anti-parallel polarized electrons on HCl molecule oriented perpendicular to the scattering plane in a coplanar geometrical arrangement.

Recently, Bhullar and Sud [13] and Sud [14] have predicted asymmetry in $(e, 2e)$ process on atoms by longitudinally polarized relativistic electrons. The longitudinal spin asymmetry in $(e, 2e)$ process on atoms has not been measured so far. Longitudinal spin asymmetry in $(e, 2e)$ process on an atom from K-shell at first sight might surprise. We present a schematic diagram of the $(e, 2e)$ ionization process on atoms in figure 1 to understand the asymmetry in $(e, 2e)$ process better. In the rest frame of the incident electron the interaction with the target electron is in the form of electromagnetic pulses (virtual longitudinal and transverse photons). The magnetic field due to the longitudinal virtual photon (B_{L}) is perpendicular to the scattering plane and the virtual transverse interaction (B_{T}) is along the direction of the beam (see figure 1b). Thus a transversely polarized electron experiences a magnetic interaction $\langle \mu_s \cdot B_{\mathrm{L}} \rangle$ and longitudinally polarized electrons $\langle \mu_s \cdot B_{\mathrm{T}} \rangle$ (see figures 1c and 1d). The asymmetry in the spin–orbit interaction for a polarized electron beam leads to asymmetry in the TDCS of the $(e, 2e)$ process on atoms. Thus longitudinal spin asymmetry in the $(e, 2e)$ process on atoms is predicted and is also expected to differ from the transverse spin asymmetry. In general, chirality in a system implies the impossibilities of overlapping of an object with its mirror image. However, chirality in $(e, 2e)$ process on K-shell of atom is due to non-overlapping of the transverse virtual photon, scattered and ejected electron with its mirror image (see figure 2). The longitudinal spin asymmetry A_{L} is defined as

$$A_{\mathrm{L}} = \frac{\mathrm{d}^3\sigma/\mathrm{d}E_1\mathrm{d}\Omega_1\mathrm{d}\Omega_2(+) - \mathrm{d}^3\sigma/\mathrm{d}E_1\mathrm{d}\Omega_1\mathrm{d}\Omega_2(-)}{\mathrm{d}^3\sigma/\mathrm{d}E_1\mathrm{d}\Omega_1\mathrm{d}\Omega_2(+) + \mathrm{d}^3\sigma/\mathrm{d}E_1\mathrm{d}\Omega_1\mathrm{d}\Omega_2(-)}, \tag{1}$$

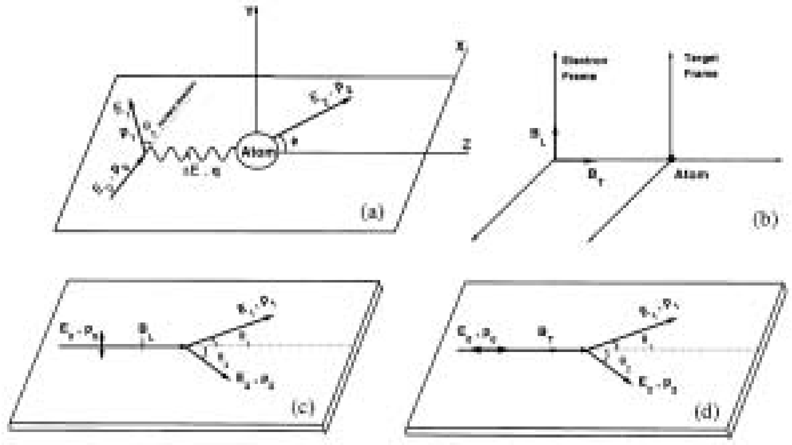

Figure 1. Schematic diagram of $(e, 2e)$ process on atoms showing (**a**) the electron–atom interaction via exchange of virtual photon energies, momenta and angles of the incoming as well as two outgoing electrons respectively indexed 0, 1 and 2, (**b**) $\mathbf{B_L}$ and $\mathbf{B_T}$ are the magnetic field due to the virtual photons in the rest frame of the electron, (**c**) spin–orbit interaction with the transversely polarized incident electrons, and (**d**) spin–orbit interaction with the longitudinally polarized incident electrons.

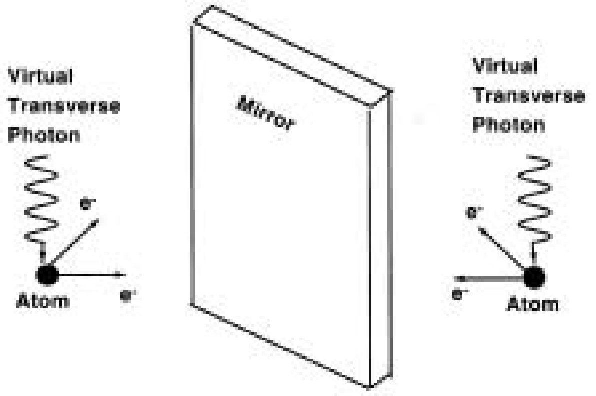

Figure 2. Chirality induced in $(e, 2e)$ process on atoms by exchange of virtual transverse photon.

where $\mathrm{d}^3\sigma/\mathrm{d}E_1\mathrm{d}\Omega_1\mathrm{d}\Omega_2(+)$ and $\mathrm{d}^3\sigma/\mathrm{d}E_1\mathrm{d}\Omega_1\mathrm{d}\Omega_2(-)$ are the triple differential cross-section for K-shell ionization for $(e, 2e)$ reaction on atoms by longitudinally polarized electron beam with polarization parallel to the beam $(+)$ and antiparallel to the beam $(-)$ respectively. Bhullar and Sud [13] developed a formalism in which S-matrix element is evaluated in one photon exchange approximation using Dirac plane waves for incident and scattered electrons. The bound K-shell and ejected electrons are represented by Darwin wave function and non-relativistic Coulomb wave function multiplied by the Darwin matrix respectively. They have shown that the longitudinal spin asymmetry for atoms in $(e, 2e)$ reaction depends on electron impact energy, atomic numbers of the target and scattered electron angle.

In this communication we present the formalism to evaluate the electron dichroism in relativistic $(e, 2e)$ process on atom in plane wave Born approximation (PWBA) using one photon exchange approximation. In the plane wave Born approximation the continuum electrons are represented by plane waves and the cross-section for the $(e, 2e)$ process can be expressed in terms of atomic structure functions, which in turn can be related to bilinear combination of the four-current components in momentum space. Donnelly [15] has given detailed formalism for decomposition of the PWBA cross-section into product of the kinematical factors and structure functions using the fact that the potential generated by the plane wave electron can be separated into the so-called longitudinal and transverse parts with respect to the momentum transfer direction. However, the high-energy approximation used here makes the TDCS for the $(e, 2e)$ process on K-shell of the atom to be expressible in terms of the atomic structure functions. Further, the longitudinal spin asymmetry has been analytically discerned in terms of kinematic factors and the interference between transition atomic charge and the component of the transition current in the direction perpendicular to the scattering plane. In §2 we briefly present the theoretical model used for $(e, 2e)$ process on atoms using one photon exchange approximation to evaluate the TDCS $(\mathrm{d}^3\sigma/\mathrm{d}E_1\mathrm{d}\Omega_1\mathrm{d}\Omega_2)$ for K-shell ionization and spin asymmetry A_L by longitudinally polarized relativistic electron beam. In §3 we present the results of our calculation of TDCS and longitudinal spin asymmetries for Al, Cu, Ag and Au targets by electron impact at energies 300 and 500 keV.

2. Theory

In this section we present the outline of the plane wave Born approximation (PWBA) theory to compute the TDCS by the longitudinally polarized electrons for $(e, 2e)$ process on atom. We choose the laboratory frame of reference in which the atom is at the origin of the coordinate system. We show the kinematics of the $(e, 2e)$ process on atom in figure 1, in which $P_0^\mu \equiv (E_0, \mathbf{P}_0)$ and $P_1^\mu \equiv (E_1, \mathbf{P}_1)$ are the four momenta of the incident and scattered electrons respectively. These two electrons are in the x–z plane $(\varphi = 0)$, and the scattered electron makes an angle θ_1 with the incident electron beam axis. The ejected electron has four momenta $P_2^\mu \equiv (E_2, \mathbf{P}_2)$ with its direction described by solid angle $\mathrm{d}\Omega_2 \equiv (\theta_2, \varphi_2)$ and $q^\mu \equiv (\Delta E, \mathbf{q})$ denotes four momentum transfer in the Z-direction. In the plane wave Born approximation the TDCS for $(e, 2e)$ process on atom by longitudinally polarized electron following Donnelly [15] can be expressed in the laboratory frame as

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}E_1\mathrm{d}\Omega_1\mathrm{d}\Omega_2} = \frac{2\pi}{I_\mathrm{in}}\rho_{e_1}\rho_{e_2} \cdot \frac{1}{4}\left[\frac{4\pi\pi}{q_\mu^2}\right]^2 \cdot \eta^{\mu\nu}W_{\mu\nu}, \tag{2}$$

where I_in is the incident electron flux given by P_0/E_0 and α is the fine structure constant. The density of states ρ_{e_1} and ρ_{e_2} have the same form for both the outgoing electrons and are given by the Fermi phase space as

$$\rho_{e_i} = \frac{P_i E_i}{(2\pi)^3}; \quad i = 1, 2. \tag{3}$$

The electron tensor ($\eta^{\mu\nu}$) and atomic tensor ($W_{\mu\nu}$) have the form as

$$\eta^{\mu\nu} = \sum_{s_0, \pm s_1} |\bar{u}^{s_1}(P_1)\gamma^{\mu}\bar{u}^{s_0}(P_0)|^* \cdot |\bar{u}^{s_1}(P_1)\,\gamma^{\mu}\bar{u}^{s_0}(P_0)| \tag{4}$$

and

$$W_{\mu\nu} = \sum_{s_2, s_b} J_{\mu}^* \cdot J_{\nu}, \tag{5}$$

where s are the spin projections with respect to the quantization axis which we take to be the incident electron beam direction and $u's, \gamma's$ and $J_\mu \equiv (J_0, \mathbf{J})$ are electron spinors, Dirac matrices and atomic transition four currents respectively.

Using the contraction of the electron and atomic tensors, the TDCS for longitudinally polarized electron on an unpolarized target is given as

$$\begin{aligned}\frac{\mathrm{d}^3\sigma(\pm)}{\mathrm{d}E_1\mathrm{d}\Omega_1\mathrm{d}\Omega_2} = \frac{P_2E_2}{(2\pi)^3}\sigma_{\mathrm{m}}[&V_{\mathrm{L}}W_{\mathrm{L}} + V_{\mathrm{T}}W_{\mathrm{T}} + V_{\mathrm{TT}}W_{\mathrm{TT}}\cos 2\phi \\ &+V_{\mathrm{LT}}W_{\mathrm{LT}}\cos\phi \pm V_{\mathrm{LT}'}W_{\mathrm{LT}'}\sin\phi],\end{aligned} \tag{6}$$

where σ_{m} is the well-known Mott cross-section; $V_{\mathrm{L}}, V_{\mathrm{T}}, V_{\mathrm{TT}}, V_{\mathrm{LT}}$ and $V_{\mathrm{LT}'}$ are electron kinematic factors and are explicitly given as

$$\begin{aligned}&V_{\mathrm{L}} = \frac{q_{\mu}^4}{q^4}, \quad V_{\mathrm{T}} = \left(\tan^2\frac{\theta_1}{2} - \frac{q_{\mu}^2}{2q^2}\right), \quad V_{\mathrm{TT}} = -\frac{q_{\mu}^2}{2q^2}\cos 2\phi, \\ &V_{\mathrm{LT}} = -\left(\frac{q_{\mu}^2}{q^2}\tan^2\frac{\theta_1}{2} - \frac{q_{\mu}^2}{q^2}\right)^{1/2}\cos\phi \quad \text{and} \quad V_{\mathrm{LT}'} = -\frac{q_{\mu}^2}{q^2}\tan\frac{\theta_1}{2}\sin\phi.\end{aligned} \tag{7}$$

The quantities $W_{\mathrm{L}}, W_{\mathrm{T}}, W_{\mathrm{TT}}, W_{\mathrm{LT}}$ and $W_{\mathrm{LT}'}$ are the longitudinal, transverse, transverse–transverse, longitudinal–transverse and polarization longitudinal–transverse atomic structure functions, respectively, and are defined in terms of the components of $W_{\mu\nu}$ and are given here in terms of the components of the atomic transition four current as

$$\begin{aligned}&W_{\mathrm{L}} = W_{00} = J_0J_0^*, \quad W_{\mathrm{T}} = W_{11} + W_{22} = J_x^*J + J_y^*J, \\ &W_{\mathrm{TT}} = W_{11} - W_{22} = J_x^*J - J_y^*J, \\ &W_{\mathrm{LT}} = -(W_{01} + W_{10}) = -2\,\mathrm{Re}[J_0^*J_x^*] \text{ and} \\ &W_{LT'} = -(W_{02} + W_{20}) = -2\,\mathrm{Re}[J_0^*J_y].\end{aligned} \tag{8}$$

The separation in eq. (6) in the form has been possible in high-energy approximation. We can express the longitudinal spin asymmetry A_{L} (eq. (1)) by using eqs (1) and (6) as

$$A = \frac{2V_{\mathrm{LT'}} W_{\mathrm{LT'}} \ \sin\phi}{V_{\mathrm{L}} W_{\mathrm{L}} + V_{\mathrm{T}} W_{\mathrm{T}} + V_{\mathrm{TT}} W_{\mathrm{TT}} \ \cos 2\phi + V_{\mathrm{LT}} W_{\mathrm{LT}} \cos\phi}. \tag{9}$$

The atomic structure function $W_{\mathrm{LT'}}$ is the interference between the transition charge J_0 and the component of the transition current in the direction perpendicular to the scattering plane. The explicit expression for $W_{\mathrm{LT'}}$ is given as $W_{\mathrm{LT'}} = -\sqrt{2}\,\mathrm{Re}\,[J_0^* J_y]$.

In the next section we present the results of our study of electron dichroism effects in the relativistic $(e, 2e)$ process for K-shell ionization of atoms in non-coplanar asymmetric geometry.

3. Results and discussion

The triply differential cross-section for K-shell ionization of atoms by relativistic unpolarized incident electrons have been computed by a number of workers in Coulomb Born approximation [16–19], relativistic first Born approximation [20–22], relativistic Coulomb Born approximation [23,24] and relativistic distorted wave Born approximation [25,26]. In the computational technique used by the workers [16–26] the incident and scattered electrons have been represented by any one of the following form: Dirac plane waves or Coulomb wave or a distorted Coulomb function with spin polarization projection perpendicularly up or down the scattering plane. Further, if the average is done over the incident electron spin projection quantum numbers one gets the TDCS due to the unpolarized electrons from the unpolarized targets. The calculation based on theories [16–26] broadly explain the shape, position and shifting of binary peak away from the direction of the momentum transfer of the experimental TDCS of K-shell ionization in coplanar asymmetric as well as in other geometrical arrangements. In Bhullar and Sud [13] and in the present investigation the incident electrons are represented by Dirac plane wave which is also a simultaneous eigenfunction of the helicity operator. In the present investigation the TDCS of K-shell ionization for $(e, 2e)$ reaction by unpolarized electrons is obtained by taking the average of the TDCS due to the longitudinally polarized electron beam with spin polarization parallel and antiparallel to the beam (eqs (6) and (9)). We present in figures 3a–c the results of our calculation of the TDCS for K-shell ionization of atoms (Cu, Ag and Au) by unpolarized incident electron beam ($E_0 = 300$ keV, $\theta_1 = -9°$) in coplanar asymmetric geometry. It is found that our calculation reproduces the shape and position of the binary peak for all the three targets. The recoil peak structure is formed but the agreement is not so good.

We present the results of our calculation of TDCS for K-shell ionization of atoms (by using eq. (6)) by unpolarized incident electron beam as well as longitudinal spin asymmetry (by using eq. (9)) for Al, Cu, Ag and Au targets in non-coplanar asymmetric geometry in figure 4. The calculation has been done for incident electron energy 300 keV for azimuthal angles $\phi = 22°, 45°, 67°$ and $90°$ at scattering angle $\theta_1 = -9°$. The TDCS by unpolarized incident electrons in non-coplanar asymmetric geometry show binary as well as recoil peak structure similar to the one observed in coplanar asymmetric geometry. Experimental data as well as theoretical results from other techniques are not available. We have shown in figure 4 (in figures 4e–4h) longitudinal asymmetry in non-coplanar asymmetric geometry

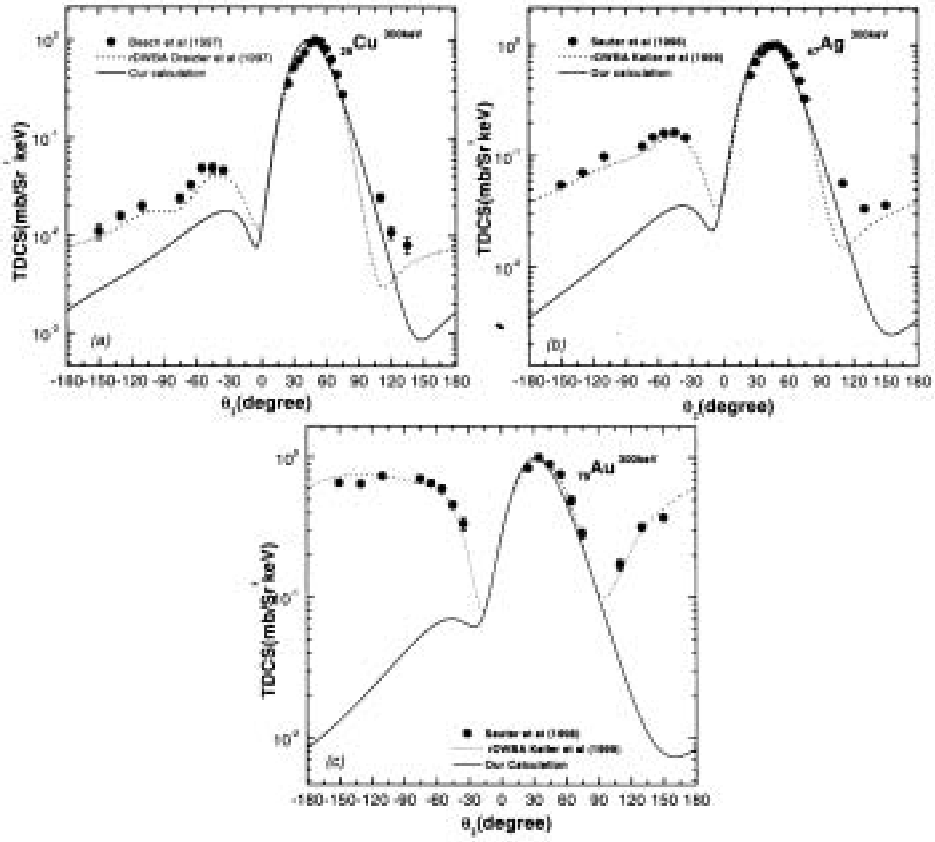

Figure 3. Relative TDCS for electron impact ionization cross-section as a function of emission angle of the slow electron (θ_2) in non-coplanar asymmetric geometries: $E_0 = 300$ keV, $E_2 = 71$ keV, $\theta_1 = -9°$ on (**a**) Cu, (**b**) Ag and (**c**) Au targets. Symbols: experimental data of Besch *et al* [27] (Cu) and Sauter *et al* [28] (Ag and Au), dashed curve: relativistic DWBA calculation of Dreizler *et al* [29] and Keller *et al* [30] and full curve: present calculation for unpolarized incident electron beam.

for scattering angle $\theta_1 = -9°$ in TDCS of K-shell ionization of Al, Cu, Ag and Au as a function of ejected electron angle θ_2 for azimuthal angles $\phi = 22°, 45°, 67°$ and 90°. The predicted longitudinal asymmetry is large and oscillatory. It is found to vary with the atomic number of the target as well as incident electron energy. The same behaviour of longitudinal spin asymmetry is observed at incident electron energy 500 keV but for brevity we have not shown the calculation here.

The present investigation on $(e, 2e)$ process on atoms by relativistic electrons shows that the longitudinal spin asymmetry in non-coplanar asymmetric geometry is large, measurable and varies with the incident electron impact electron energy, atomic number and ejected electron angle. In the present formalism longitudinal spin asymmetry in TDCS of K-shell ionization cross-section for any target is zero

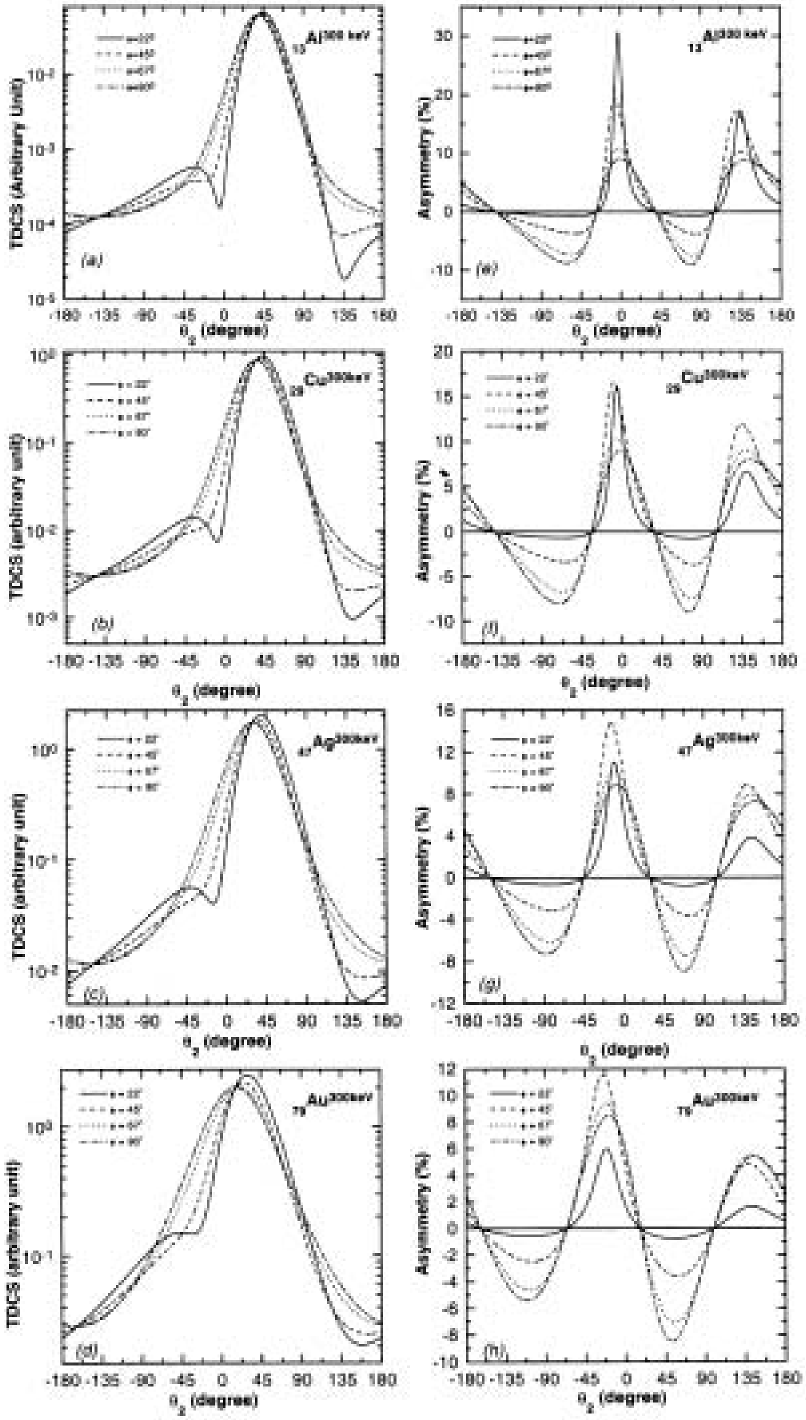

Figure 4. TDCS K-shell ionization cross-section as a function of emission angle of the slow electron (θ_2) in non-coplanar asymmetric geometries: $E_0 = 300$ keV, $E_2 = 71$ keV, $\theta_1 = -9°$ on (**a**) Al, (**b**) Cu, (**c**) Ag and (**d**) Au for different azimuthal angles ($\phi = 22°, 45°, 67°$ and $90°$). The calculated longitudinal spin asymmetry for the kinematics of (a), (b), (c) and (d) are shown in (**e**), (**f**), (**g**) and (**h**) respectively.

in coplanar geometry (i.e. $\phi = 0°$, see eq. (9)). This is expected as the TDCS of the $(e, 2e)$ process on atom into the product of electronic and atomic tensors (eq. (2)) is possible only in the extreme relativistic limit (i.e. $m_e = 0$) and chirality of the interaction in the $(e, 2e)$ processes in this approximation in the coplanar arrangement is not present. The spin polarized cross-section is found to depend on the ejected electron angle θ_2. It is also observed that the longitudinal spin asymmetry is zero at four ejected electron angles (θ_2) and further at these points it is also independent of the azimuthal angle ϕ. At these points the TDCS for the process with the electron spin polarized along the beam direction as well as opposite to it is equal. The position of each zero depends on the atomic number, energy of the target as well as the electron impact energies. More sophisticated calculations and experiments will help us to understand the spin polarized electron ionization process better. The spin asymmetry is also found to depend on the electron impact energy and is large at lower electron impact energy. The longitudinal spin asymmetry has been computed by evaluating the interference term between the transition charge and the component of the transition current (eq. (9)) in the direction perpendicular to the scattering plane and the kinematical structure function. The dependence of A_{L} on energy is through two factors in an involved way. It is further found that the ejected electron angle θ_2 at which longitudinal spin asymmetry A_{L} is zero do not change with the azimuthal angle.

Our calculation of TDCS explains the shape, position and shifting of the binary peak away from the direction of the momentum transfer (figure 3). As the spin asymmetry is a relative difference between the triple differential cross-sections for K-shell ionization of atoms for $(e, 2e)$ reaction on atom by longitudinally polarized electrons with spin polarization being parallel and antiparallel to the beam, it may have a better agreement with the experiment as compared to TDCS. However, through the present investigation we have demonstrated the electron dichroism effects as well as the role of virtual transverse interaction in the relativistic $(e, 2e)$ process on atom. Unfortunately, no experiment has been performed so far for the relativistic $(e, 2e)$ process on atoms by using longitudinally polarized beam. It would be interesting to have it, as this will help us to understand the process better.

Further, we conclude with the remarks that our study has shown that the $(e, 2e)$ process on atom in non-coplanar geometry provides a tool to probe the interference between the transition charge and transverse transition current. We suggest more theoretical investigation in distorted wave Born approximation of the longitudinal spin asymmetry in the relativistic $(e, 2e)$ process in non-coplanar as well as coplanar geometry. We further suggest that experimental measurements of the longitudinal spin asymmetry be undertaken to further understand the role and importance of the spin polarized $(e, 2e)$ studies.

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