PRAMANA
— journal of
physics

Vol. 63, No. 5
November 2004
pp. 977–991

Electron impact excitation of the *D* states of Mg, Ca and Sr atoms: Complete experiment results

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MS received 24 December 2003; revised 27 June 2004; accepted 31 July 2004

Abstract. We have used non-relativistic and relativistic distorted wave approximation methods to study the excitation of the $n\,^1D$ states of magnesium ($n = 3$), calcium ($n = 4$) and strontium ($n = 5$) from the ground $n\,^1S$ state. Calculations have been performed for the complete set of parameters $(\sigma, \tilde{L}_\perp^+, \tilde{L}_\perp^-, \tilde{\gamma}^+, \tilde{\gamma}^-)$. The results are presented for electron impact energies of 20 and 40 eV. We compare our results obtained from both the non-relativistic and relativistic methods with each other. Good agreement is found on comparison and the importance of relativistic effects is also explored.

Keywords. Electron; excitation; atoms; complete experiment.

PACS Nos 34.80.Dp; 34.80.Nz

1. Introduction

Recently there has been an increased activity for studying excitation of atoms by electron impact with the special emphasis on achieving a 'complete scattering experiment' [1,2], which would result in the determination of all the quantum mechanical scattering amplitudes that define the process. Such studies have been analyzed in considerable detail for the excitation of light and heavy atoms from an S-state (orbital angular momentum $L = 0$) to a P-state ($L = 1$) [3–6]. Similar studies for the excitation to a D state ($L = 2$) are quite challenging for both theorists and experimentalists because the complete description in this case requires more independent scattering parameters and the scattered electron-single photon coincidence experiments do not allow for unique determination of the complex scattering amplitudes. Instead a triple coincidence experiment (which involves coincidence detection between the scattered electron and two photons emitted in the subsequent decay of the atom from $D \to P$ and then $P \to S$) is required [3,7–9]. Due to these complexities, up to now, study of D state excitation is confined to simpler atom like helium [3,7–9].

Through recent papers from our group [10,11], we reported differential cross-sections and Stokes parameters for the D state excitation of some alkaline earth elements like Mg, Ca and Sr. The study of alkaline earth atoms provides an opportunity to investigate the general transition from light to heavy atoms while maintaining the s^2 closed outer shell structure. In the present paper we extend our work on the D state excitation of alkaline earth atoms in view of a 'complete scattering experiment'. So far the complete experiment study has been achieved only for the excitation of helium from its ground ^1S state to the $3\,^1D$ state at 40 eV. We report here the complete experiment parameters for the excitation from $n\ ^1S$ state to the $n\ ^1D$ state of Mg ($n = 3$), Ca ($n = 4$) and Sr ($n = 5$). Though there are no experimental data to compare with our results, we have carried out two types of calculations, viz. relativistic distorted wave (RDW) and non-relativistic distorted wave (DW) approximation methods. The results obtained from these two methods are compared with each other. Thus the importance of relativistic effects in these atoms is also explored.

In §2 we first discuss the parametrization of the complete quantum mechanical description of the process of a D state excitation and describe the complete experiment parameters. Section 3 briefly outlines the calculations. In §4 all the results are presented.

2. Theory

If the fine structures of the atomic states are not resolved, the excitation of an atom from the state i having initial orbital angular momentum L_i to the final state f having orbital angular momentum L_f by impact of electrons having energy (momentum) $E_i(\mathbf{k_i})$ can be described at a fixed scattering angle by the scattering amplitudes $f(L_f, M_{L_f}, \mathbf{k_f}; L_i, M_{L_i}, \mathbf{k_i})$, defined by

$$f(L_f, M_{L_f}, \mathbf{k_f}; L_i, M_{L_i}, \mathbf{k_i}) = (2\pi)^2 \left(\frac{k_f}{k_i}\right)^{1/2} T_{i\to f}(L_f, M_{L_f}, \mathbf{k_f}; L_i, M_{L_i}, \mathbf{k_i}), \tag{1}$$

where $\mathbf{k_f}$ is the momentum of the scattered electron, $T_{i\to f}$ is the transition matrix and M_{L_i}, M_{L_f} are the z-components of the orbital angular momentum L_i and L_f respectively. Here the normalization of the scattering amplitudes has been done according to the definition that the square modulus gives differential cross-section, i.e. $\sigma(L_f, M_{L_f}, L_i, M_{L_i}) = |f|^2$.

In specific case of excitation of an atom from the S state to the D state (i.e. $L_i = 0 \to L_f = 2$), the scattering amplitudes that define the process are $f(2, M_{L_f}, \mathbf{k_f}; 0, 0, \mathbf{k_i})$ with $M_{L_f} = 2, 1, 0, -1, -2$. For the sake of brevity, hereafter these amplitudes will be denoted by $f_{M_{L_f}}$. If we consider 'natural frame of reference' then the scattering amplitudes for $M_{L_f} = 1, -1$ vanish due to their reflection symmetry along the scattering plane and the process can be completely described by only three amplitudes, i.e. f_2, f_0 and f_{-2}, which can be expressed as

$$f_2^{\mathrm{n}} = \alpha_2 \mathrm{e}^{i\phi_2}, \tag{2a}$$

$$f_0^{\mathrm{n}} = \alpha_0 \mathrm{e}^{i\phi_0}, \tag{2b}$$

$$f_{-2}^{\mathrm{n}} = \alpha_{-2} \mathrm{e}^{i\phi_{-2}}. \tag{2c}$$

Superscript 'n' denotes the natural frame of reference and α_2, α_0 and α_{-2} are the magnitudes and ϕ_2, ϕ_0 and ϕ_{-2} are the phases of the scattering amplitudes.

2.1 *Complete experiment parameters*

For complete description of the S–D excitation process by electron impact, in addition to the differential cross-section (DCS), the magnitudes of two scattering amplitudes with $M_{L_f} = \pm 2$ and their relative phases with respect to the scattering amplitude with $M_{L_f} = 0$ must be determined [3,7]. In this way one can determine completely the scattering amplitudes given by eqs (2a)–(2c). Consequently, besides the measurement of DCS, other experimental techniques like electron–photon coincidence experiments to measure remaining quantities are needed.

In electron–photon coincidence experiments, the polarization of the photon emitted after the decay of the excited atom to a lower state is analysed in coincidence with the scattered electron. For example, after excitation to the D state of an atom by electron impact, the excited atom can decay to a lower P state through a photon emission, which subsequently decays further to a lower S state by the emission of a second cascading photon. Therefore the scattered electron–emitted photon coincidence experiment can be performed by detecting the scattered electrons in coincidence with either of the emitted photons. These experiments measure the Stokes parameters P_i $(i = 1-4)$, where P_i $(i = 1, 2, 3)$ are measured perpendicular to the scattering plane and P_4 is measured in the scattering plane.

$$P_1 = \frac{I(0^\circ) - I(90^\circ)}{I(0^\circ) + I(90^\circ)}, \tag{3a}$$

$$P_2 = \frac{I(45^\circ) - I(135^\circ)}{I(45^\circ) + I(135^\circ)}, \tag{3b}$$

$$P_3 = \frac{I(\mathrm{RHC}) - I(\mathrm{LHC})}{I(\mathrm{RHC}) + I(\mathrm{LHC})}, \tag{3c}$$

where $I(\beta^\circ)$ is the intensity of the light transmitted by the detector placed perpendicular to the scattering plane and having its transmission axis in the direction β° with respect to the incident electron direction. $I(\mathrm{RHC})$ and $I(\mathrm{LHC})$ are the intensities of the right- and left-handed circularly polarized light components as detected by the circular polarization analyser placed perpendicular to the scattering plane. Further, P_4 is given by

$$P_4 = \frac{I(0^\circ) - I(90^\circ)}{I(0^\circ) + I(90^\circ)}. \tag{3d}$$

Here $I(\beta^0)$ is the intensity of the light transmitted by the detector placed in the scattering plane and having its transmission axis in the direction β^0 with respect to the incident electron direction.

The maximum information that can be obtained from such a scattering experiment (i.e. scattered electron–single photon coincidence) can be expressed in terms of the parameters $L_\perp, h, \gamma$ and P_ℓ, defined as [6]

$$L_\perp = -2P_3(1-h), \tag{4a}$$

$$h = \frac{(1+P_1)(1-P_4)}{4-(1-P_1)(1-P_4)}, \tag{4b}$$

$$P_\ell \mathrm{e}^{2i\gamma} = P_1 + iP_2, \tag{4c}$$

where $L_\perp$ is the angular momentum transferred perpendicular to the scattering plane, γ is the alignment angle of charge cloud of the excited D state, h is the height of charge cloud and P_ℓ is the linear polarization. However, through such experiment all the four parameters needed for the complete description, i.e. two relative magnitudes and two relative phases cannot be determined. It leads to the determination of two relative sizes of the amplitudes through the values of $L_\perp$ and h that can be obtained from (4a) and (4b) but it leads two solutions (values) for the relative phases.

Therefore, for the complete determination of the scattering amplitudes, a triple coincidence experiment [3,7–9] is required in which scattered electron is detected in coincidence with both the photons emitted through the $D \to P$ and $P \to S$ decay processes. If we consider the decay of the D state, through $D \to P \to S$, it should be noted that for the detection of emitted photon in the z-direction (i.e. perpendicular to the scattering plane, in natural frame), the transition with $M_L = 0$ are not observable. Thus the two decay paths in the optical decay pattern $D \to P \to S$ may be distinguished by the sublevel $M_L = \pm 1$ of the P-level [7]. These paths may be characterized by the helicity (+ or −) of the subsequent $P \to S$ cascading photon. Thus the measurements of the Stokes parameters $P_1^\pm, P_2^\pm, P_3^\pm$ and $P_4^\pm$ (where the superscript refers to the two possible channels) for the two channels are made by detecting the polarization of the emitted $D \to P$ photon in coincidence with the scattered electron and the circular polarization analysis of $P \to S$ photon. $P_1^\pm, P_2^\pm, P_3^\pm$ and $P_4^\pm$ are as defined in eqs (3a)–(3d) measured when the helicity of $P \to S$ photon is '+' or '−'.

The information so obtained from the triple coincidence experiments can be expressed in terms of the parameters $\tilde{L}_\perp^+, \tilde{L}_\perp^-, \tilde{\gamma}^+, \tilde{\gamma}^-$ defined as

$$\tilde{\gamma}^\pm = \tan^{-1}\left(\frac{P_2^\pm}{P_1^\pm}\right), \tag{5a}$$

$$\tilde{L}_\perp^\pm = -2P_3^\pm(1-\tilde{h}^\pm), \tag{5b}$$

where

$$\tilde{h}^\pm = \frac{(1+P_1^\pm)(1-P_4^\pm)}{4-(1-P_1^\pm)(1-P_4^\pm)}. \tag{5c}$$

Thus the complete experiment parameters can be expressed as (σ, $\tilde{L}_\perp^+$, $\tilde{L}_\perp^-$, $\tilde{\gamma}^+$, $\tilde{\gamma}^-$) including the differential cross-section. Once the parameters $P_1^\pm, P_2^\pm, P_3^\pm, P_4^\pm$

are measured from the scattered electron-emitted two-photon coincidence experiments along with the DCS measurement, the description of S–D excitation is complete.

Theoretically the complete parameter set can be obtained through the following relations:

$$\sigma = \alpha_2^2 + \alpha_0^2 + \alpha_{-2}^2, \tag{6a}$$

$$\tilde{L}_\perp^\pm = \pm 2 \frac{\alpha_{\pm 2}^2 - \frac{1}{6}\alpha_0^2}{\alpha_{\pm 2}^2 - \frac{1}{2}\alpha_0^2}, \tag{6b}$$

$$\tilde{\gamma}^\pm = \pm\pi - \delta_{\pm 2} \quad \text{where } \delta_{\pm 2} = \pm(\phi_{\pm 2} - \phi_0), \tag{6c}$$

where α_2, α_0 and α_{-2} and $\phi_{\pm 2}$, ϕ_0 are as defined in eqs (2a)–(2c).

2.2 *Distorted wave approximation method*

To evaluate the complete experiment parameters theoretically, as defined by eqs (6a)–(6c), all scattering amplitudes which are connected to the transition matrix through eq. (1) are required to be calculated. The T-matrix for the electron impact excitation of an atom (having N electrons and nuclear charge Z) from an initial state i to final state f in distorted wave approximation can be written as (atomic units are used throughout)

$$T_{i\to f}^{\mathrm{DW}} = \langle \chi_f^-(1, 2, \ldots, N+1) | V - U_f(N+1) | \chi_i^+(1, 2, \ldots, N+1) \rangle, \tag{7}$$

where V the target–projectile interaction, is given by

$$V = -\frac{Z}{r_{N+1}} + \sum_{j=1}^{N} \frac{1}{|\mathbf{r_j} - \mathbf{r_{N+1}}|}. \tag{8}$$

Here $\mathbf{r_j}$ $(j = 1,\ 2, \ldots, N)$ is the position coordinate of the target electrons and $\mathbf{r_{N+1}}$ is the position coordinate of projectile electron with respect to the nucleus of the atom. U_f is the distortion potential which is taken to be a function of radial coordinates of the projectile electron only, i.e. r_{N+1}. Also U_f is chosen to be a spherically averaged static potential of the excited state of atoms. This choice of U_f has been shown to yield most consistent results [12–14].

The wave function $\chi_{i(f)}^{+(-)}$ is represented as a product of target N-electron wave function $\phi_{i(f)}$ and projectile electron distorted wave function $F_{i(f)}^{\mathrm{DW}+(-)}$, i.e.

$$\chi_{i(f)}^{+(-)}(1, 2, \ldots, N+1) = A\phi_{i(f)}(1, 2, \ldots, N) F_{i(f)}^{\mathrm{DW}+(-)}(\mathbf{k_{i(f)}}, N+1), \tag{9}$$

where A is the antisymmetrization operator that takes into account the contribution of the exchange of projectile electron with the target electrons.

In non-relativistic distorted wave theory the wave function $\phi_{i(f)}$ of the target atom are taken to be the solution of the Schrödinger equation,

$$H_{\text{atom}}\phi_{i(f)} = \varepsilon_{i(f)}\phi_{i(f)}, \tag{10}$$

where

$$H_{\text{atom}} = \sum_{j=1}^{N}\left(-\frac{Z}{r_j} - \frac{\nabla_j^2}{2}\right) + \sum_{i<j}^{N}\frac{1}{|\mathbf{r_i} - \mathbf{r_j}|} \tag{11}$$

and $\varepsilon_{i(f)}$ is the eigenenergy of the target atom. The wave function $\phi_{i(f)}$ is usually chosen to be Hartree–Fock-type. In non-relativistic distorted wave theory the projectile distorted electron wave function satisfies the following equation:

$$\left[-\frac{1}{2}\nabla_{N+1}^2 + U_{i(f)}\right] F_{i(f)}^{\text{DW}} = E_{i(f)}F_{i(f)}^{\text{DW}}. \tag{12}$$

We expand the distorted wave $F^{\text{DW}+(-)}$ using the following general non-relativistic form of partial wave expansion:

$$F^{+(-)}(\mathbf{k},\mathbf{r}) = \frac{1}{\sqrt{k}}\sum_{\ell=0}^{\infty}(2\ell+1)i^{\ell}\mathrm{e}^{\pm i\delta_{\ell}(k^2)}\frac{u_{\ell}^{\pm}(k,r)}{r}P_{\ell}(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}), \tag{13}$$

where δ_ℓ is the phase shift of the ℓth partial wave, P_ℓ is Legendré polynomial of order ℓ and $u_\ell^{\pm}(k,r)$ is the radial part of the distorted wave function. On substituting expression for $F^{+(-)}$ as given above in eq. (13) into eq. (12) we get

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{\ell(\ell+1)}{r^2} + 2U(r)\right] u_\ell(k,r) = 0 \tag{14}$$

which is solved numerically subject to the following usual boundary conditions

$$u_\ell(k,r) \underset{r\to 0}{=} 0 \tag{15}$$

and

$$u_\ell(k,r) \underset{r\to\infty}{=} \frac{1}{\sqrt{k}}\sin\left[kr - \frac{1}{2}\ell\pi + \delta_\ell(k^2)\right]. \tag{16}$$

2.3 *Relativistic distorted wave method*

In relativistic distorted wave method, the wave function $\phi_{i(f)}$ of the target atom is taken to be the solution of the Dirac equation, i.e. eq. (10) with,

$$H_{\text{atom}} = \sum_{j=1}^{N}[-ic\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}_{\mathbf{j}} + \beta c^2 + V_{\text{nuc}}(r_j)] + \sum_{i<j}^{N}\frac{1}{|\mathbf{r_i} - \mathbf{r_j}|}, \tag{17}$$

where α and β are Dirac matrices and $-i\nabla_j$ represents the momentum operator of the jth target electron and $V_{\text{nuc}}(r_j) = -Z/r_j$. The wave function of the bound

state of N-electron atom, i.e. $\phi_{i(f)}$, is generally chosen to be a Slater determinant of single Dirac–Fock orbitals which are given by

$$\phi_{n\kappa m}(\mathbf{r},\sigma) = \frac{1}{r}\begin{pmatrix} P_{n\kappa}(r)\chi_{\kappa m}(\hat{r},\sigma) \\ Q_{n\kappa}(r)\chi_{-\kappa m}(\hat{r},\sigma) \end{pmatrix}, \tag{18}$$

where $P_{n\kappa}$ and $Q_{n\kappa}$ are large and small components of radial wave functions and $\chi_{\pm\kappa m}$ represents the spin-angular wave function, given by

$$\chi_{\kappa m}(\hat{\mathbf{r}},\sigma) = \sum_{\mu\nu}\left(\ell\mu\frac{1}{2}\nu\middle|jm\right)Y_{\ell\mu}(\hat{\mathbf{r}})\psi_{(1/2)\nu}(\sigma) \tag{19}$$

and

$$\chi_{-\kappa m}(\hat{\mathbf{r}},\sigma) = \sum_{\mu\nu}\left(\tilde{\ell}\mu\frac{1}{2}\nu\middle|jm\right)Y_{\tilde{\ell}\mu}(\hat{\mathbf{r}})\psi_{(1/2)\nu}(\sigma), \tag{20}$$

where j is the total angular momentum of the orbital, m is the z-component of j, $\tilde{\ell} = 2j-\ell, (\ell_1 m_1 \ell_2 m_2|\ell_3 m_3)$ represent Clebsch–Gordan coefficient and $\psi_{(1/2)\nu}(\sigma)$ are normalized spin wave functions.

It should be noted that spin- and orbital-angular momenta are coupled together. The spin-angular state is characterized by quantum number κ, which is defined as

$$\kappa = \begin{cases} \ell, & \text{if } \; j = \ell - 1/2 \;\; \text{for } \ell > 0 \\ -\ell - 1, & \text{if } \; j = \ell + 1/2 \end{cases}. \tag{21}$$

The bound state orbital satisfy the following orthogonality conditions:

$$\int_0^\infty \mathrm{d}r[P_{n'\kappa}(r)P_{n\kappa}(r) + Q^{(r)}_{n'\kappa}Q^{(r)}_{n\kappa}] = \delta_{n'n} \tag{22}$$

and

$$\langle\chi_{\kappa m}(\hat{r},\sigma)|\chi_{\kappa' m'}(\hat{r},\sigma)\rangle = \delta_{\kappa'\kappa}\delta_{m'm}. \tag{23}$$

We express the energy relativistically by $E_{i(f)} = (\frac{1}{2}k^2_{i(f)}c^2 + c^4)^{1/2}$. Here c is the velocity of light. Further, we use for the projectile electron distorted wave function $F^{\mathrm{DW}}_{i(f)}$ the following relativistic form of partial wave expansion:

$$F^{\pm}_{\mathrm{ch},\mu_{\mathrm{ch}}}(\mathbf{k}_{\mathrm{ch}},\mathbf{r}) = \frac{1}{(2\pi)^{3/2}}\sum_{\kappa m}\mathrm{e}^{\pm i\eta_\kappa}a^{\mu_{\mathrm{ch}}}_{\mathrm{ch},\kappa m}(\hat{k}_{\mathrm{ch}})\frac{1}{r}\begin{pmatrix} f_\kappa(r)\chi_{\kappa m}(\hat{r}) \\ ig_\kappa(r)\chi_{-\kappa m}(\hat{r}) \end{pmatrix} \tag{24}$$

with

$$a^{\mu_{\mathrm{ch}}}_{\mathrm{ch},\kappa m}(\hat{k}_{\mathrm{ch}}) = 4\pi i^l\left[\frac{E_{\mathrm{ch}}+c^2}{2E_{\mathrm{ch}}}\right]^{1/2}\sum_{m_l}\left(lm_l\frac{1}{2}\mu_{\mathrm{ch}}\middle|jm\right)Y^*_{lm_l}(\hat{k}_{\mathrm{ch}}). \tag{25}$$

Here 'ch' refers the two channels, i.e. initial i and final f. $\mu_{\rm ch}$ is the spin projection of the projectile electron and η_κ is the phase shift of the partial wave. The radial parts $f_\kappa(r)$ and $g_\kappa(r)$ are the solutions of the following integro-differential equations:

$$\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\kappa}{r}\right)f_\kappa(r)-\frac{1}{c}(c^2-U+E_{\rm ch})g_\kappa(r)-\frac{1}{cr}W_Q(\kappa;r)=0, \tag{26}$$

$$\left(\frac{\mathrm{d}}{\mathrm{d}r}-\frac{\kappa}{r}\right)g_\kappa(r)+\frac{1}{c}(-c^2-U+E_{\rm ch})f_\kappa(r)+\frac{1}{cr}W_P(\kappa;r)=0, \tag{27}$$

with boundary conditions

$$f_\kappa(r)\underset{r\to\infty}{\longrightarrow}\sin\left(k_{\rm ch}r-\frac{l\pi}{2}+\eta_\kappa\right), \tag{28a}$$

$$g_\kappa(r)\underset{r\to\infty}{\longrightarrow}\frac{c}{c^2+E_{\rm ch}}\cos\left(k_{\rm ch}r-\frac{l\pi}{2}+\eta_\kappa\right). \tag{28b}$$

W_P and W_Q in the above equations are the non-local exchange kernels as discussed by McEachran and Stauffer [15]. These integro-differential equations are solved numerically as described by Zuo [16]. It should be noted that the spin of the target as well as the projectile electrons naturally enters in the description through Dirac equations in RDW method. Also the spin- and orbital-angular momentum are coupled together and form spin-angular state which is defined by total angular momentum j or κ. Therefore the RDW method gives the scattering amplitudes for the transition from the state having total angular momentum J_i to the state having total angular momentum J_f, i.e. it gives scattering amplitude for the fine-structure resolved transitions. For example, if we denote the states of the target atom in LS coupling scheme, the theory gives the scattering amplitude for transition from the state $^{2S_i+1}L_{f_{J_i}}$ to the state $^{2S_f+1}L_{f_{J_f}}$.

3. Theoretical calculations

3.1 *The RDW calculation*

We first describe our calculations of the complete parameters in the RDW method. In the relativistic j–j coupling notation, the ground state configurations of Mg, Ca and Sr are $1s^22s^22\bar{p}^22p^43s^2$, $1s^22s^22\bar{p}^22p^43s^23\bar{p}^23p^44s^2$ and $1s^22s^22\bar{p}^22p^43s^23\bar{p}^23p^43\bar{d}^43d^64s^24\bar{p}^24p^45s^2$ respectively. The valence shell of these atoms have configuration ns^2 ($n=3$ for Mg, $n=4$ for Ca, $n=5$ for Sr). Therefore the ground state of the atoms Mg, Ca, Sr have total angular momentum $J_i=0$ and can be represented as $n\ ^1S_0$ in LS-coupling scheme. For the excited D states, the outer shell involves configurations of the form $nsn'\bar{d}$ with $J_f=1,2$ or $nsn'd$ with $J_f=2$ or 3 where $n'=3,4$ and 5 for Mg, Ca and Sr respectively. These states can be represented as $n'\ ^1D_2$ and $n'\ ^3D_{1,2,3}$ with even parity in LS-coupling scheme. We have considered in this paper the excitation of $n\ ^1D_2$ state only.

The configuration of the $^1S_0$ and $n\ ^1D_2$ states are taken to be the same type of multiconfiguration ground state (MCGS) calculation as in Muktavat *et al* [10] (for Ca and Sr) and Srivastava et al [11] (for Mg). The Grasp92 program of Parpia *et al* [17] is used to calculate the Dirac–Fock orbitals. The transition matrix is then evaluated using eq. (7) after calculating the distorted wave functions. The details of the method for evaluating T-matrix for atoms having two electrons in their valence shell are given in Kaur *et al* [18].

The RDW scattering amplitudes, which give transition between fine-structure resolved states are then transformed to the fine structure unresolved amplitudes $f_{M_{L_f}}$ defined in eq. (1) using the following formula:

$$f_{M_{L_f}} = \sum_{M_{S_i} M_{S_f} \mu_i \mu_f} \sum_{J_i J_f M_i M_f} \left(SM_S \middle| S_f M_{S_f} \frac{1}{2} \mu_f \right) (L_f M_{L_f} S_f M_{S_f} | J_f M_f) \times (J_i M_i | L_i M_{L_i} S_i M_{S_i}) \left(S_i M_{S_i} \frac{1}{2} \mu_i \middle| SM_S \right) f(J_f M_f \mu_f; J_i M_i \mu_i), \tag{29}$$

where $S_i, S_f, M_{S_i}, M_{S_f}$ are the spin-angular momenta and their z-components of the target atom. J_i, J_f, M_i, M_f are the total angular momenta and their z-components of the target states. The total spin of target projectile system S and its z-component M_S are conserved, i.e.

$$M_S = M_{S_i} + \mu_i = M_{S_f} + \mu_f. \tag{30}$$

It should be noted that the calculation of T-matrix is first performed in 'collision frame of reference' for convenience. Therefore, the scattering amplitudes obtained using eq. (1) remains in 'collision frame of reference'. These amplitudes are transformed into natural frame of reference amplitudes using the following transformation relations:

$$f_2^n = -\frac{1}{4} f_{-2}^c - \frac{i}{2} f_{-1}^c + \sqrt{\frac{3}{8}} f_0^c + \frac{i}{2} f_1^c - \frac{1}{4} f_2^c, \tag{31a}$$

$$f_0^n = -\sqrt{\frac{3}{8}} f_{-2}^c - \frac{1}{2} f_0^c - \sqrt{\frac{3}{8}} f_2^c, \tag{31b}$$

$$f_{-2}^n = -\frac{1}{4} f_{-2}^c + \frac{i}{2} f_{-1}^c + \sqrt{\frac{3}{8}} f_0^c - \frac{i}{2} f_1^c - \frac{1}{4} f_2^c. \tag{31c}$$

Here the superscript 'c' refers to the collision frame of reference. The natural frame scattering amplitudes obtained from the above transformation relations are then used to calculate the complete parameters defined in eqs (6a)–(6c).

3.2 *The DW calculation*

Similarly, in order to evaluate the non-relativistic T-matrix and hence the complete parameters, first we require the wave function for the target atom in its initial and

final states. The Hartree–Fock wave function has been used to represent bound states of the atoms. These wave functions are obtained using Fischer's code [19]. Thereafter the distortion potential and distorted waves are obtained to calculate the T-matrix finally. The details of these calculations for atoms having two valence electrons are given in [20].

4. Results and discussion

We performed the calculations for obtaining the complete parameters for the excitation of Mg, Ca and Sr from their ground state $n\ ^1S$ to the excited $n\ ^1D$ state ($n = 3$ for Mg, $n = 4$ for Ca and $n = 5$ for Sr) by electron impact at 20 and 40 eV. We do not have any other theoretical or experimental data to compare with our calculations. We therefore compare the two types of calculations we performed, i.e. using DW and RDW methods.

We show our DW and RDW results of the differential cross-sections at 20 and 40 eV in figures 1, 2 and 3, respectively for the Mg, Ca and Sr atoms. The experimental data are available only for the DCS of Mg which are also shown in figure 1. These experimental data are taken from [21]. The DCS for the calculation of the singlet states considered here show forward peak in all the cases, which is a typical characteristic of an allowed transition. In all the figures DW and RDW results show similar type of variations. The RDW results for the DCS of Mg at 20 and 40 eV show better agreement with the experimental data when compared to DW results and thus reflect the importance of relativistic effects in the excitation process. Similar to Mg the RDW and DW results for Sr are also in reasonable agreement. However, the two results for Ca are not in good agreement with each other quantitatively at both the energies, through the shapes of their DCS curve are somewhat similar. This could be due to the choice of wave functions [10].

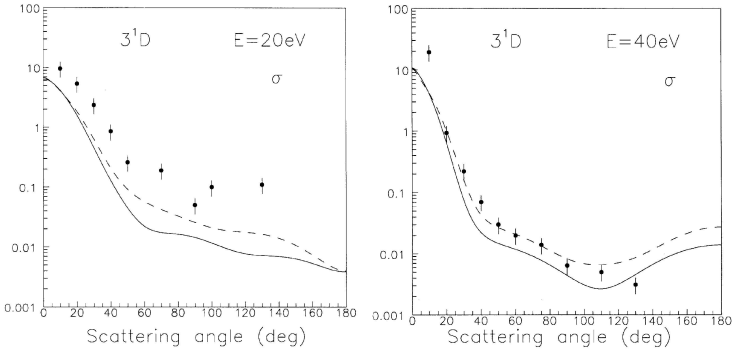

Figure 1. Differential cross-sections in atomic units for the excitation of the $3\ ^1D$ state of Mg atom by electron impact at 20 and 40 eV. — DW; - - - RDW; • experiment [21].

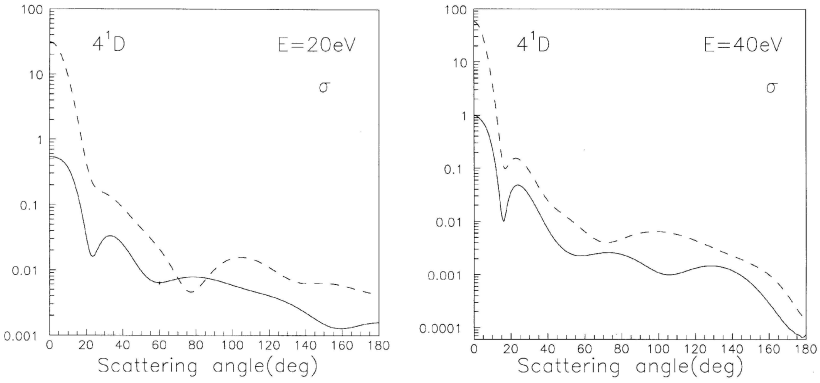

Figure 2. Same as in figure 1 but for the excitation of the 4 ^1D state of Ca atom.

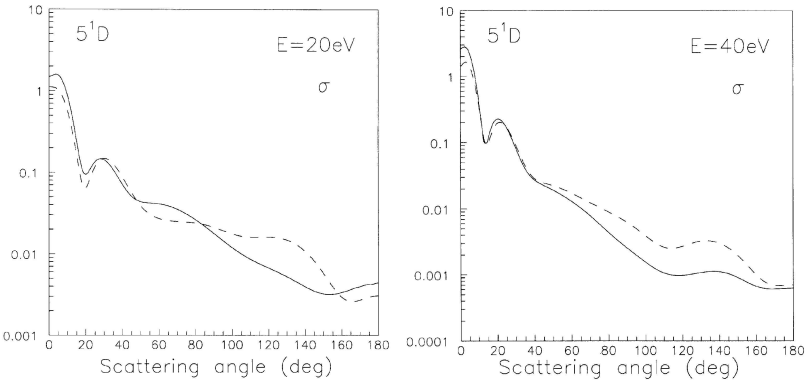

Figure 3. Same as in figure 1 but for the excitation of the 5 ^1D state of Sr atom.

Through figures 4–9 we have shown the other complete parameter results $(\tilde{L}_\perp^+, \tilde{L}_\perp^-, \tilde{\gamma}^+, \tilde{\gamma}^-)$ at energies 20 and 40 eV for Mg, Ca and Sr atoms. We first compare the results for the parameters $\tilde{L}_\perp^+$ and $\tilde{L}_\perp^-$ for Mg, Ca and Sr atom which are shown in the figures. According to the first Born approximation prediction (FBA) of Andersen and Bartschat [7], in the forward direction the parameters $\tilde{L}_\perp^+ = \tilde{L}_\perp^- = 4/3$. It is seen that for the three atoms, similar to helium, the parameters $\tilde{L}_\perp^+$ and $\tilde{L}_\perp^-$ do not vanish for the forward and backward scattering angles, instead they have the same limiting values as predicted by Andersen and Bartschat [7] in the FBA. We see that for Mg at scattering angle $\sim$110° the parameter $\tilde{L}_\perp^\pm \approx \pm 2$, where according to eq. (6b) α_0^2 vanishes thereby giving rise to $\tilde{L}_\perp^\pm \approx \pm 2$. For Sr, this feature arises near about 150° scattering angle and for Ca it arises for scattering angle $\sim$160°. In all the cases RDW and DW results are in good agreement with each other.

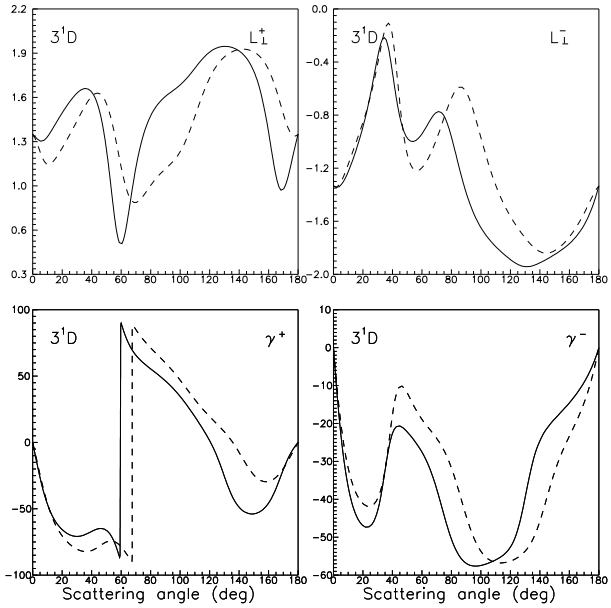

Figure 4. Complete set of parameters $\tilde{L}_{\perp}^{+}, \tilde{L}_{\perp}^{-}, \tilde{\gamma}^{+}$ (in degrees), $\tilde{\gamma}^{-}$ (in degrees) for the excitation of the $3\ ^1D$ state of Mg atom by electron impact at 20 eV. Figure captions are the same as in figure 1.

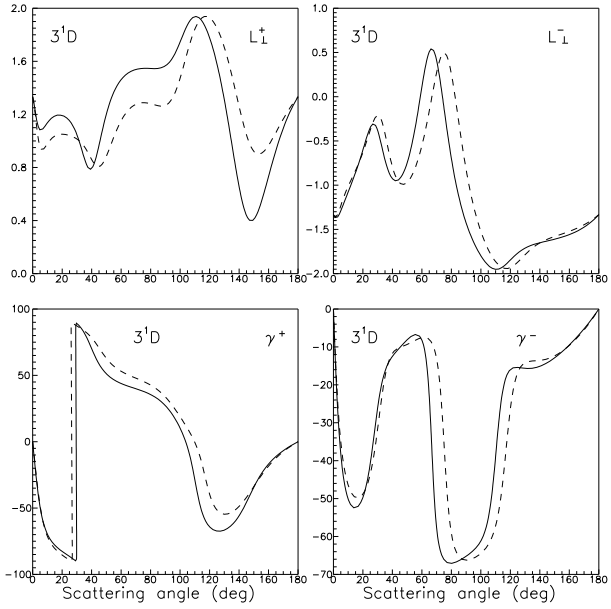

Figure 5. Same as in figure 4 but at 40 eV.

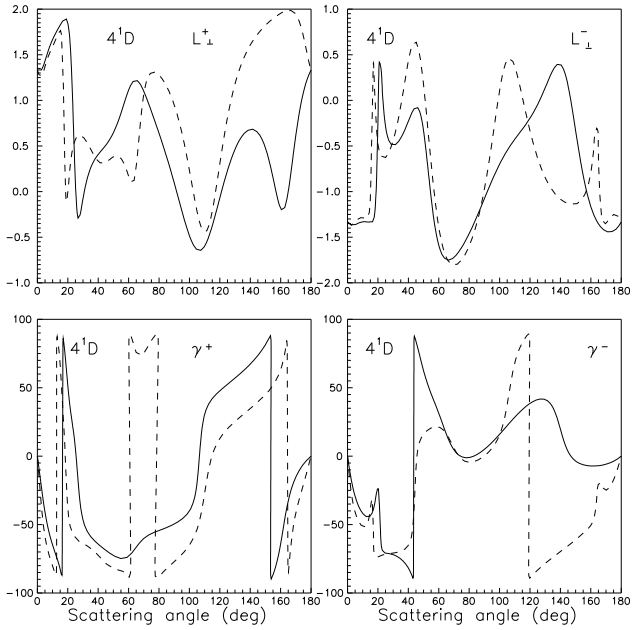

Figure 6. Same as in figure 4 but for the excitation of the 4 ^1D state of Ca atom.

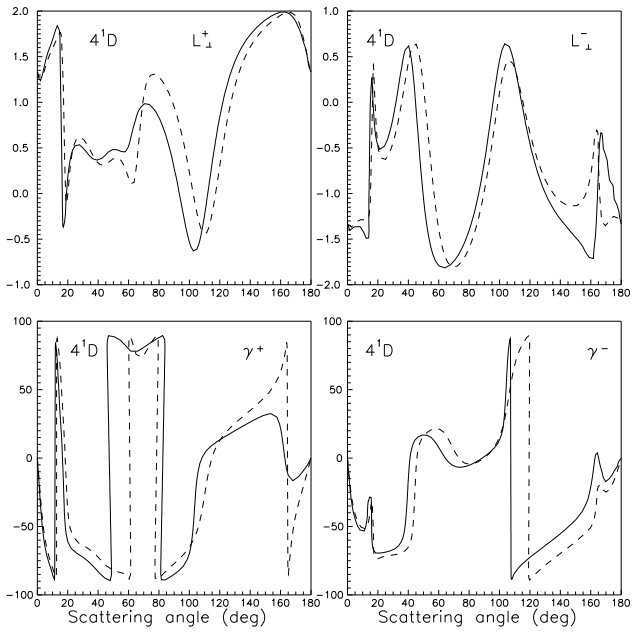

Figure 7. Same as in figure 5 but for the excitation of the 4 ^1D state of Ca atom.

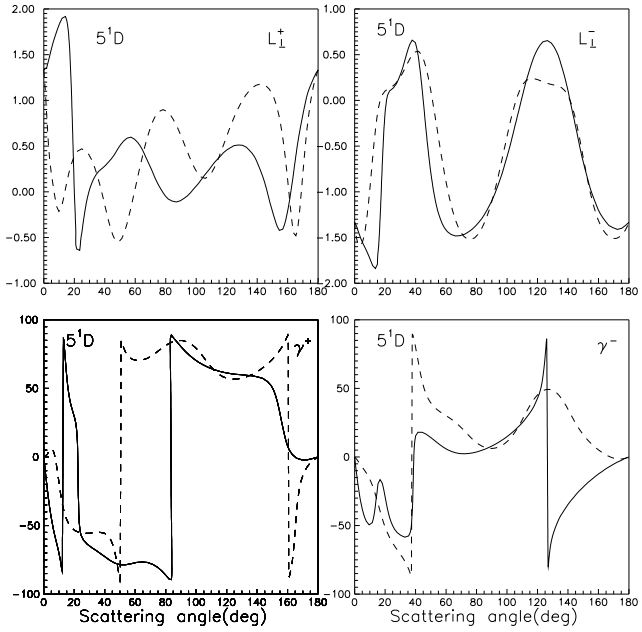

Figure 8. Same as in figure 4 but for the excitation of the 5 ^1D state of Sr atom.

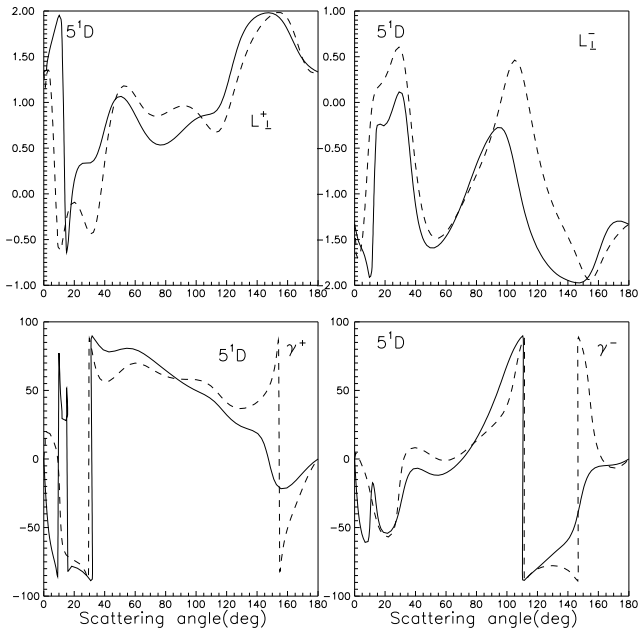

Figure 9. Same as in figure 5 but for the excitation of the 5 ^1D state of Sr atom.

We next compare the $\tilde{\gamma}^+$ and $\tilde{\gamma}^-$ results for Mg, Ca and Sr atoms as shown in these figures. We see that $\tilde{\gamma}^+ = \tilde{\gamma}^-$ in the forward and backward direction in all the cases. Here also a reasonable agreement is found between DW and RDW results.

5. Conclusion

We have reported complete experiment parameters for the excitation of the D states of the three alkaline earth atoms, viz. Mg, Ca and Sr at 20 and 40 eV. For the first time the S–D excitation of these atoms has been analysed in a complete sense. A reasonable agreement is found between the DW and RDW theories. The importance of relativistic effects is also reflected in the results. It would be interesting to have the experimental confirmation of these results.

Acknowledgements

The authors are thankful to Prof. A D Stauffer for fruitful discussions. The financial assistance from CSIR, New Delhi is gratefully acknowledged. One of the authors (SS) is thankful to CSIR for the senior research fellowship.

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