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Study of photon-induced L_3 vacancy alignment for elements La to U

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Abstract. Alignment of photon-induced L_3 vacancies is studied in rare earth and high Z elements at energies of experimental interest, near thresholds to 60 keV, under non-relativistic dipole approximation. Numerical calculations of the matrix element are undertaken to produce theoretical data for comparison with the experimental findings. The A_2 values being >0.1 at photoelectron energies <20 keV are certainly higher than 5–8% uncertainties quoted in experimental results. Present findings are from a very basic model, hydrogen-like and can further be treated as reference to observe the impact of screening, relativistic, multipole and retardation corrections to the model.

Keywords. X-ray fluorescence; vacancy alignment; magnetic sub-states; point Coulomb potential; non-relativistic dipole approximation.

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1. Introduction

Atomic inner-shell vacancies created in different modes of atomic ionization may be aligned in a vacancy state with total angular momentum $j > 1/2$. Alignment results from the fact that the ionization cross-sections of an electron with total angular momentum j have different values for different projection m_j of j on the incident photon direction. This is interpreted in terms of alignment parameter, A, as the fractional difference of magnetic sub-states (m_j's) ionization cross-sections [1–6]. So far, the inner shell alignment has been well-established for different charged particles-induced ionization processes [5]. For the first time, Flugge *et al* [1] predicted that photoionization of inner shell electrons also leads to the alignment of vacancies in the states, $j > 1/2$.

Later on, Oh and Pratt [2] calculated relative probabilities of $|m_j| = 3/2$ and $|m_j| = 1/2$ electron ejection from L_3 and M_3 sub-shells. Besides this, Berezhko *et al* [4] and Kleiman and Lohmann [6] made systematic calculations of alignment for

a number of atoms undergoing photoionization in inner shells only in the vicinity of ionization thresholds.

Direct measurements of dependence of photoeffect on magnetic sub-states are not possible but the alignment is exhibited by directional correlation and polarization of characteristic X-rays and Auger electrons emitted on decay of the vacancies. The angular measurements of L-shell X-ray fluorescence (L XRF) cross-sections following photoionization induced by 60 and 26 keV or threshold photons in some rare earth and high Z elements are available from the work of seven different groups [7–13]. First three groups [7–9] established the anisotropic distribution of L X-rays. The measured values of group II are slight and those of groups I and III are much higher than the theoretical predictions of Berezhko *et al*. Moreover, the L X-ray distribution patterns reported by groups I and II deviated from those for dipole character of X-rays, whereas, the three other groups IV, V and VI [10–12] predicted the isotropic distribution within the experimental uncertainties. Later on, group V [11] reported an anisotropy for Au L_l and L_α emissions at 13 keV that culminated in an alignment value ∼50% higher than the theoretical predictions. Recently, Barrea *et al* [13] have reported their experimental anisotropy parameter and degree of alignment, which are in very good agreement with the predicted theoretical value.

Keeping the mentioned discrepancies in view, the photon-induced L_3 vacancy alignment is studied in elements La–U at energies of experimental interest, 10 to 40 keV above the thresholds. The calculations are made using point Coulomb potential to build up atomic model and non-relativistic dipole approximation for electron wave functions in different states. The details are given in the following sections.

2. Formulation and calculations for A_2 parameter

For calculation of photon-induced inner shell vacancy alignment, all the theoretical formulations [2–6] express quantity A_2 as a function of the L_3 vacancy population $\sigma(P_{3/2}, m_j)$ as

$$A_2 = \frac{\sigma(P_{3/2}, m_j = \pm 3/2) - \sigma(P_{3/2}, m_j = \pm 1/2)}{\sigma(P_{3/2}, m_j = \pm 3/2) + \sigma(P_{3/2}, m_j = \pm 1/2)}, \tag{1}$$

where m_j is the absolute value of the magnetic quantum number. Often, the calculations of magnetic sub-state photoionization cross-section $\sigma(P_{3/2}, m_j)$ involve selection of potential to build up an atomic model and approximations regarding electron wave function.

Oh and Pratt [2] calculated the relative probabilities of $m_j = 3/2$ and $1/2$ electron ejection from L_3 and M_3 sub-shells for Ca and Mg under both relativistic Born approximation and non-relativistic dipole approximation. Besides this, Berezhko *et al* [4] and Kleiman and Lohmann [6] in their alignment calculations used independent particle model with a spherical symmetric self-consistent potential for matrix element. They have made systematic calculations of alignment for a number of atoms undergoing photoionization in inner shells, only in the vicinity of ionization thresholds, using Herman–Skillman wave functions. No doubt, the model used by Berezhko *et al* [4] and Kleiman and Lohmann [6] seems to be realistic and

appropriate, but it works better at thresholds and near thresholds where there is a probability of overlapping of atom and outgoing electron wave functions and requires finer details of the wave functions. At energies, 10 to 40 keV above thresholds, the overlapping chances are bleak or not there. Therefore, Coulomb potential to build up atomic model is the appropriate potential. Consequently, the present calculations of alignment are made using point Coulomb potential to build up atomic model and non-relativistic dipole approximation for electron wave functions in different states as

- the energy range, (threshold to 60 keV) $\ll mc^2$, satisfies the non-relativistic constraint on photon energies,
- elements in the range La to U satisfy the condition; (photon energy/mc^2) $\ll Z\alpha$ (α is the fine structure constant) that gives photon wavelength large compared to the radius of the bound electron. This supports the dipole approximation.
- The choice of Coulomb potential in the present circumstances also draws support from the statement quoted by Bechler and Pratt [14] that with increasing energy, when higher multipoles are needed, point Coulomb calculations become quite accurate.

But because of the involvement of heavy elements and higher energies in the present studies, the dipole approximation and Coulomb potential concepts are clubbed together.

In the case of inner-shell photoionization with photons of energy, k (in terms of mc^2), the matrix element for the interaction,

$$M_{\text{photo}} = \langle N, p|M|I\rangle, \tag{2}$$

where I is the initial state of the atom, N is the intermediate state (once ionized state) of the atom and p is the linear momentum of the outgoing electron.

The differential photoionization cross-section averaged over initial photon polarization comes as [2]

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = (2\pi)^2 \frac{e^2\hbar^3}{m^2ck} \sum_{\varepsilon} |M_{\text{photo}}|^2. \tag{3}$$

Under dipole approximation, for an unpolarized incident beam and an electron with orbital angular momentum l and spin projection m_j, the ratio of cross-sections for $P_{3/2}$ sub-state becomes

$$\frac{\sigma(P_{3/2}, m_j = \pm 1/2)}{\sigma(P_{3/2}, m_j = \pm 3/2)} = \frac{|R_{l-1}|^2 + \frac{19}{5}|R_{l+1}|^2}{3|R_{l-1}|^2 + \frac{21}{5}|R_{l+1}|^2}, \tag{4}$$

where $R_{l\pm1} = \int_0^\infty \mathcal{R}_{p,l\pm1} r^3 \mathcal{R}_{nl} \mathrm{d}r$ is the single particle radial integral, and $\mathcal{R}_{p,l\pm1}$ and $\mathcal{R}_{nl}$ are continuum and bound radial wave functions of the photoelectron.

The expression for the alignment parameter A_2, from relations (1) and (4) is

$$A_2 = \frac{|R_{l-1}|^2 + \frac{1}{5}|R_{l+1}|^2}{2|R_{l-1}|^2 + 4|R_{l+1}|^2}. \tag{5}$$

In point Coulomb potential [15], the normalized bound state wave function of the photoelectron is given as

$$\mathcal{R}_{nL}(r) = N_{nL} r^L \exp(-ar/n)\, {}_1F_1[L+1-n, (2L+2), 2ar/n], \tag{6}$$

where

$$N_{nL} = [(n+L)!/2n(n-L-1)!]^{1/2}(2a/n)^{L+3/2}/(2L+1)! \tag{7}$$

is the normalization constant, $a = Z\alpha$ as α is the fine structure constant, $L = l$ is the angular momentum quantum number of bound electron and ${}_1F_1$ is the confluent hypergeometric function.

For a continuum state, the normalized wave function is

$$\mathcal{R}_{p,l'}(r) = N_{pl'} r^{l'} \exp(-ipr)\, {}_1F_1(l'+1+ia/p, 2l'+2, 2ipr) \tag{8}$$

with

$$N_{pl'} = (2p)^{l'} \exp(a\pi/2p)|\Gamma(l'+1-ia/p)|/(2l'+1)!. \tag{9}$$

Here $l' = L \pm 1$ is the angular momentum of continuum state. The momentum of outgoing electron $p = \sqrt{2T}$ where T is the kinetic energy of photoelectron in terms of mc^2, i.e. $(h\nu - \text{B.E.})/mc^2$. For $2P_{3/2}$ state, $n = 2, L = 1$ and the confluent hypergeometric functions ${}_1F_1$ have been evaluated from its series expression [16]. The calculations for A_2 using eqs (5)–(9) are performed in *Mathematica* and the generated results are shown in figure 1 for some elements.

3. Results and interpretations

Present procedure of calculations is applied for the fractional L_3 magnetic substate photoionization cross-sections for Mg and Ca and the similarities between the present results and those from the work of Oh and Pratt [2] support the current procedure.

Alignment parameter A_2 is found maximum ($\sim$0.5) at energies nearly 1 keV above L_3 threshold energy for all the elements. This supports the prediction of Berezhko *et al* [4]. Moreover, the values are found decreasing with photon energy but increasing with Z. At outgoing electron energies $\sim$ (threshold to 20 keV) for most of the elements, A_2 values ($\geq$0.1) (figure 1) are certainly much higher than the lowest limit 0.05 predicted by Berezhko *et al* [4].

The variation of alignment with photon energy (figure 1) reveals that alignment is almost negligible at thresholds but show peak value at energies about 1 keV above the L_3 thresholds and afterward it decreases with energy. Generally, the ratios of $\sigma(m_j = 3/2)/\sigma(m_j = 1/2)$ at peaks have been found to be $\approx$3. For elements, $57 \leq Z \leq 80$ in the energy range $\sim$35 to 60 keV, again some peak structures are found. It is a coincidence that most of the energy region containing the peak structure extends a few keV below and above the K-edge energy of the element. For Z's > 80, there is a smooth fall in alignment from $\sim$0.5 near the threshold energies to $\sim$0.1 at 60 keV. The prominence of alignment around K-edges may be due to the

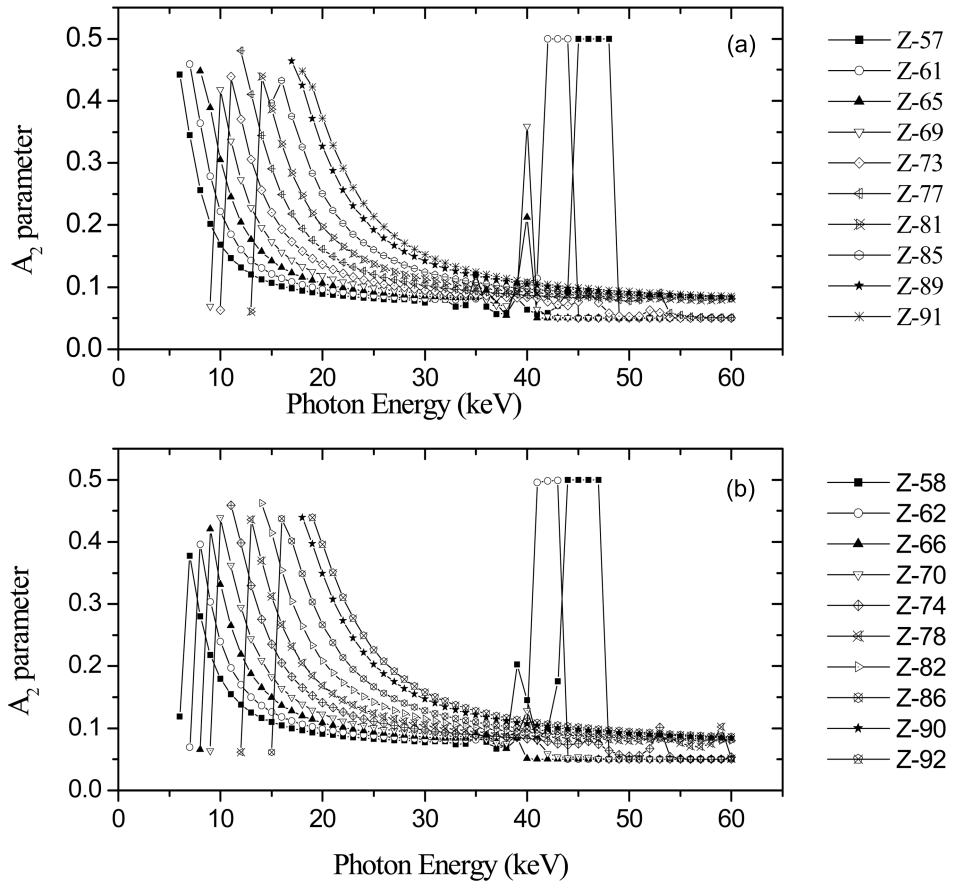

Figure 1. Plot of alignment parameter A_2 vs. photon energy for elements, (**a**) $Z = 57$, 61, 65, 69, 73, 77, 81, 85, 89 and 91 and (**b**) $Z = 58$, 62, 66, 70, 74, 78, 82, 86, 90 and 92.

disturbance of point Coulomb potential with the start of K-shell ionization. For elements with $Z > 80$, the K-edge energies >85 keV seem to support the absence of A_2 peak structure up to 60 keV. However, the intermediate results of the present calculation point towards the dominance of radial wave function R_{l+1} over R_{l-1} at thresholds and around 1 keV above thresholds the dominance of R_{l+1} and R_{l-1} reverses. A similar exchange of dominance takes place wherever the peak structure is observed near the K-edge energies.

Moreover, the A_2 values being >0.1 at electron energies <20 keV are certainly higher than 5–8% uncertainty quoted in experimental results. Further, corrections to the evaluated alignment values for intra-shell Coster–Kronig probabilities result in a conclusion supported by groups IV–VI. Hence, the distribution measurements after applying compensation for Coster–Kronig probabilities may produce alignment comparable with the present theoretical values. The measured values of groups I and III are far greater than the present results. Near threshold, for the

element Er, the alignment value of Papp and Campbell [8] is nearly compatible with the present predictions while that of Barrea *et al* [13] is lower than the present one.

4. Conclusions

Present alignment parameter calculations involving the partial photoionization of $m_j = 1/2$ and $m_j = 3/2$ states used the simplest possible atomic model, point Coulomb potential, and non-relativistic dipole approximation for electron wave function. The outcomes are: (i) almost all the results for elements $57 \leq Z \leq 92$ support the maximum 0.5 and the minimum 0.05 as A_2 limits quoted by Berezhko *et al* [4], (ii) the trends of variation in alignment parameter with energy for rare earth and high Z elements are similar to the earlier reported variation of A_2 for Mg and Ca by Oh and Pratt [2]. The A_2 values being >0.1 at energies <20 keV are certainly higher than 5–8% uncertainties quoted in experimental results. Further corrections to the evaluated alignment values for intra-shell Coster–Kronig probabilities result in a conclusion supported by groups IV–VI. The presence of energy pockets where alignment is comparatively prominent requires further exploration either with the precise measurements of low intensity L X-rays (L_l and $L_{\alpha 2}$) or by modifications of theoretical evaluations. McEnnan *et al* [17] have already pointed out that at distances smaller on the atomic scale (Compton wavelength distances) but still outside the nucleus, the atomic screening modifies the normalization of the electron wave function but the shape of the electron wave function remains Coulombic. At somewhat larger distances, i.e. energies away from thresholds, the modifications of the shape of the wave function due to screening become appreciable. Moreover, in the considered energy range at higher energies the contribution of quadrupole photoabsorption may be significant [11]. Therefore, the basic data need further check for effect of atomic screening, retardation and relativity on alignment calculations.

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