

## Methods to Determine Photon Induced Vacancy Alignment in Atomic Inner-shells

**ABSTRACT :** As alignment is fractional difference of magnetic sub-state ( $j_z$ ) ionization cross-sections, thus, these cross-sections based upon different models and assumptions have been used to determine alignment parameter ( $A_2$ ). Vacancy alignment also results in anisotropic distribution of x-rays originated from the state; therefore, the distribution measurements of the x-rays lead to  $A_2$  determination. Moreover, the magnetic sub-state ionization cross-sections of an orbital electron lead to projectile energy dependence of x-rays. The determination of  $A_2$  from these methods is being discussed here.

Photon induced atomic inner-shell vacancies in a state with  $j > 1/2$  may be aligned<sup>1</sup> i.e. the magnetic sub-states of the state may have unequal population of vacancies. The fractional photo-ionization cross-section difference from magnetic sub-states  $j_z = 3/2$  and  $1/2$  is called alignment parameter,  $A_2$ . So far, the inner shell alignment has been well established for different charged particles induced ionization processes<sup>2</sup>.

For the first time, Flugge *et al.*<sup>1</sup> explored that photo-ionization of inner shell electrons also leads to the alignment of vacancies in the states,  $j > 1/2$ . Later on, some systematic calculations of alignment for a number of atoms undergoing photo-ionization in inner shells have been made<sup>3-5,6</sup>. The experimental work on alignment in some rare earth and high Z elements is available from eight different group of workers<sup>7</sup>. The explanations regarding the origin of vacancy alignment in L3 state and its influences on subsequent processes led to different methods for alignment determination :

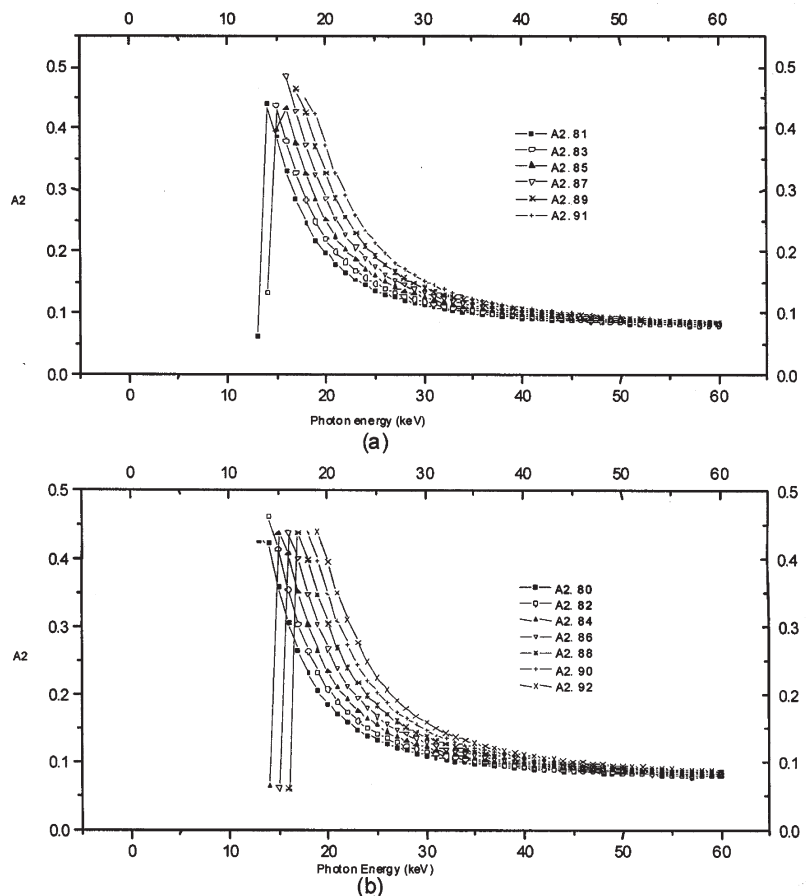
- Calculation from theoretical formulations.
- Determination from angular distribution measurements.
- Determination from production cross-section ratio for  $L\alpha$  and  $L\beta$  groups of x-rays.

**Methods to determine photon induced vacancy alignment :** (i) **Theoretical formulations :** Theoretical formulations for calculations of photon induced inner shell vacancies alignment have been developed by Oh and Pratt<sup>3</sup>, Berezhko and Kabachnik<sup>4</sup>, Berezhko *et al.*<sup>5</sup> and Kleiman and Lohmann<sup>6</sup>. The quantity  $A_2$ , as a function of the L3 vacancy population ( $\sigma^i L3(j_z)$ ), is expressed as

$$A_2 = \frac{\sigma^i L3(j_z = \pm 3/2) - \sigma^i L3(j_z = \pm 1/2)}{\sigma^i L3(j_z = \pm 3/2) + \sigma^i L3(j_z = \pm 1/2)} \quad (1)$$

where  $j_z$  is the absolute value of the magnetic quantum number taking the incident direction as the z axis. Often, the calculations of magnetic sub-state photo ionization cross section ( $\sigma^i L3(j_z)$ ) involve

- selection of potential to build up an atomic model and
- Approximations regarding electron wave function.



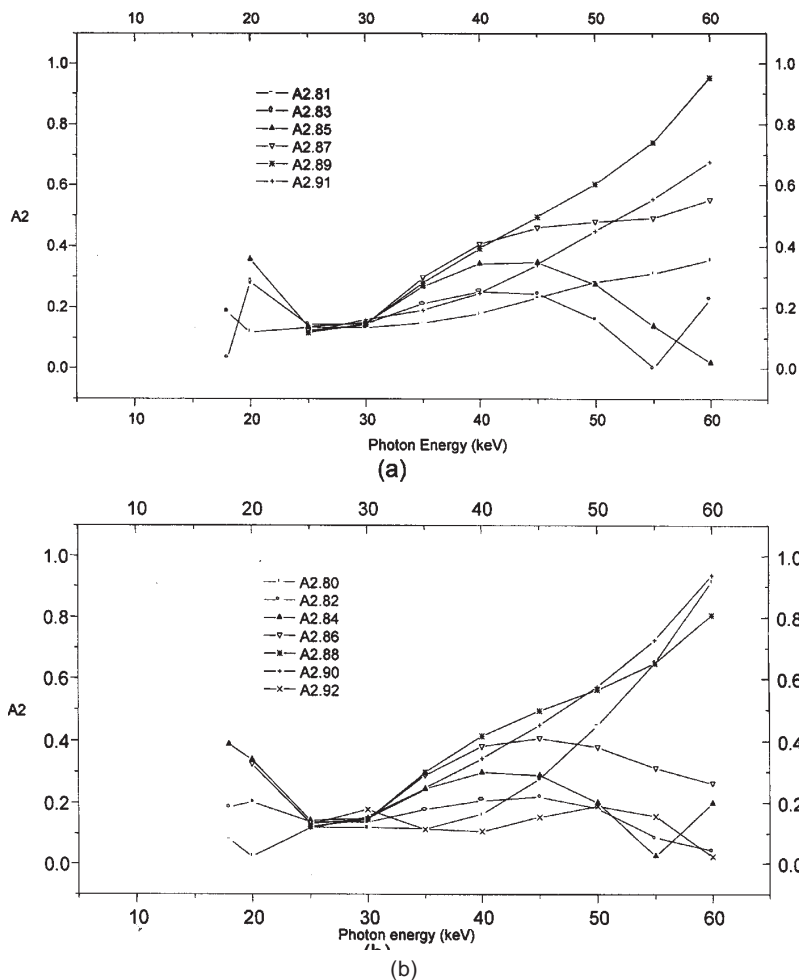
**Fig. 1.** Plot of theoretical alignment parameter  $A_2$  vs. photon energy for elements, (a)  $Z = 81, 83, 85, 87, 89$  and  $91$ ; (b)  $Z = 80, 82, 84, 86, 88, 90$  and  $92$ .

With the existing experimental set-ups and equipment, the experimental measurements are possible only in high Z elements and most of the measurements are for photon energies, threshold to 60 keV. The model used by Berezhko *et al.*<sup>5</sup>; Kleiman and Lohmann<sup>6</sup> seems to be more realistic and appropriate, but it is tedious to apply it at energies 10 to 40 keV above thresholds. Thus, attempts have been made for theoretical evaluations<sup>8</sup> of  $A_2$  for some of the elements Hg to U at different energies, thresholds to 60 keV (figure 1).

**(ii) Angular distribution measurements :** The alignment of vacancies results in anisotropy distribution of x-rays originating from the filling of the vacancies. The angular distribution  $W_L(\theta)$  of x-rays from aligned vacancies is given as

$$W_L(\theta) = W_L / 4\pi [1 + \lambda A_2 P_2(\cos \theta)] \quad (2)$$

Where  $W_L$  is the total intensity of x-rays in  $4\pi$  solid angle.  $P_2(\cos \theta)$  is the second order Legendre function,  $\theta$  is the



**Fig. 2.** Plot of empirical (Mann *et al.*) alignment parameter  $A_2$  vs. photon energy for elements, (a)  $Z = 81, 83, 85, 87, 89$  and  $91$ ; (b)  $Z = 80, 82, 84, 86, 88, 90$  and  $92$ .

angle between incident photon and emitted x-ray beam and  $\lambda$  is a constant whose value depends upon the angular momentum  $j$  of the initial and final states involved in the x-ray emission. Berezhko and Kabachnik<sup>4</sup> calculated the value of  $\lambda$  parameter in the single particle model for different transitions. Thus, experimental distribution measurements of x-rays originating from filling of the aligned vacancies can be used for evaluation of alignment parameter.

**(iii) Production cross-sections ratio of  $L\alpha$  and  $L\ell$  groups of x-rays :** Since  $L\alpha$  and  $L\ell$  x-ray lines arise from a vacancy in  $L3$  state, therefore, the energy dependence of ratio of production cross-section of these two lines if exists, it predicts alignment of vacancies in the state. The ratio can be used to determine alignment parameter.

According to Berezhko and Kabachnik<sup>4</sup>, angular distributions  $W_L(\theta)$  of  $L\alpha_1, L\alpha_2$  and  $L\ell$  x-rays emitted from aligned atoms are expressed by

$$W_{L\alpha_1}(\theta) = W_{L\alpha_1} / 4\pi [1 + 0.1 A_2 P_2(\cos \theta)] \quad (3)$$

$$W_{L\alpha_2}(\theta) = W_{L\alpha_2} / 4\pi [1 + 0.1 A_2 P_2(\cos \theta)] \quad (4)$$

$$W_{L\ell}(\theta) = W_{L\ell} / 4\pi [1 + 0.5 A_2 P_2(\cos \theta)] \quad (5)$$

$W_L$ , total intensity of each x-ray line, is proportional to the total  $L3$ -vacancy population cross section and the radiative transition probability. Therefore, the intensity ratio  $L\alpha/L\ell$  as production cross-section ratio  $\sigma_{L\alpha_{1,2}}/\sigma_{L\ell}$  is given as

$$\frac{\sigma_{L\alpha_{1,2}}(\theta)}{\sigma_{L\ell}} = \frac{W_{L\alpha_1}(\theta) + W_{L\alpha_2}(\theta)}{W_{L\ell}(\theta)} \quad (6)$$

At emission angle  $90^\circ$ , taking  $F_{3\alpha_2}/F_{3\alpha_1} = 1/9$  for hydrogen like wave functions of  $2d$  and  $2p$  states,

$$\frac{\sigma_{L\alpha_{1,2}}(90^\circ)}{\sigma_{L\ell}} = \frac{F_{3\alpha_1} + F_{3\alpha_2}}{F_3} [1 + 0.225 A_2] \quad (7)$$

Thus, the ratio  $\sigma_{L\alpha_{1,2}}/\sigma_{L\ell}$  is a function of the degree of alignment  $A_2$  as well as of radiative transition probabilities  $F$ 's and is independent of the source and mode of vacancy production. To apply this method for  $A_2$  determinations in elements Hg to U at incident photon energies, threshold

to 60 keV, the experimental LXRF cross-section  $\sigma_{L\alpha}$  ( $g = \alpha, \beta$ ) values<sup>9</sup> available for 9 elements are considered. The experimental values along with reported 8% errors are interpolated using the computer software IGELCS<sup>10</sup>. The ratios along with the values of radiative decay rates Scofield<sup>11</sup> are used to calculate  $A_2$  in relation (7). The plot of  $A_2$ 's (magnitudes) versus incident photon energy is shown in figure 2.

### Conclusion

The outcomes of first and third method for evaluations of  $A_2$  supports the maximum 0.5 and minimum 0.05 limits quoted by Berezhko *et al.*<sup>5</sup>. The comparison of the data with the empirical evaluated values supports the trend of variations of  $A_2$  with energy, except for the disparities at higher energies. This requires either the precise measurements of low intensity  $L\beta$  and  $L\alpha_2$  x-rays or modifications of theoretical evaluations with atomic screening, retardation and relativity etc. corrections.  $\square$

AJAY SHARMA#  
AND RAJ MITTAL<sup>1</sup>

#Physics Department, Chitkara University,  
Barotiwala (Solan)  
H. P.-174 103, India

<sup>1</sup>Nuclear Science Laboratories, Physics Department,  
Punjabi University, Patiala 147 002, India

E-mail: ajay.sharma@chitkarauniversity.edu.in

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- <sup>1</sup> S. Flugge, W. Mehlhorn and V. Schmidt, *Phys. Rev. Lett.* **29**, 7 (1972).
- <sup>2</sup> D. Bhattacharya, *Ind. J. Phys.* **B69**, 83 (1995)
- <sup>3</sup> S. D. Oh and R. H. Pratt, *Phys. Rev.* **A10**, 1198 (1974)
- <sup>4</sup> E. G. Berezhko and N. M. Kabachnik, *J. Phys.* **B10**, 2467 (1977)
- <sup>5</sup> E. G. Berezhko, N. M. Kabachnik and V. S. Rostovsky, *J. Phys.* **B11**, 1749 (1978)
- <sup>6</sup> U. Kleiman and B. Lohmann, *J. Elect. Spectro. and Rel. Phen.* **131** 29 (2003)
- <sup>7</sup> A. Sharma, R. Mittal, In the proceedings of DAE-BRNS symposium on atomic, molecular and optical Physics (NCAMP-XVII) IUAC, New Delhi, 135 (2009), R. Mittal and Vandana, *Rad. Phys. Chem.* **51**, 357 (1998)
- <sup>8</sup> A. Sharma, M. Singh and R. Mittal, *Pramana* **66** 1111 (2006)
- <sup>9</sup> K. S. Mann, N. Singh, R. Mittal, B. S. Sood and K. L. Allawadi, *X-ray Spectrom* **23** 208 (1994)
- <sup>10</sup> R. Mittal, M. Singh and Vandana, *X-ray Spectrom* **32** 285 (2003)
- <sup>11</sup> J. H. Scofield, *At. Data Nucl. Data Table* **14** 121 (1974)