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Coster-Kronig Corrected Experimental and Theoretical Alignment Parameter for Tungsten-a Comparison

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An attempt has been made to study the effect of Coster-Kronig (CK) fij correction on alignment parameter (A20) calculated by measuring angular distribution of L x-rays of tungsten (W) in the angular range 0° to 120° at 17.781 keV, the energy that is above L1 edge of W where CK transitions shift the vacancies from L1 and L2 states to L3 state. The experimental CK corrected alignment parameter is compared with the same calculated using non-relativistic dipole approximation in a point Coulomb potential. It is found that the value of alignment is increased by ~32 % of its value by including this CK correction in experimental calculations.

Key Words: Alignment parameter, Coster-Kronig transitions, angular measurements and non-relativistic dipole approximation.

INTRODUCTION

For photon induced processes, Flugge *et al.*[1] were the first to explore the alignment of inner shell vacancies. Numerical calculations of vacancy alignment have been performed with different approaches, but some systematic numerical calculations are provided by Berezhko *et al.*[2] and Kleiman and Lohmann[3]. Up to date survey of literature reveals that since eighties the experimental alignment measurements of L x-ray fluorescence cross-sections following photo-ionization in some rare earth and high Z elements are available from the work of eight different groups[4] and predicted contradictory results. To sort out the ambiguity among the results from angular measurements and alignment parameter calculations, an attempt has been made to study the effect of CK correction on alignment parameter calculated by measuring angular measurements of L x-rays of W in the angular range 0° to 120° at 17.781 keV that is above L1 edge of W where CK transitions shift the vacancies from L1 and L2 states to L3 state.

EXPERIMENTAL

The measurements are performed in XRF laboratories of Raja Ramanna Center of Advanced Technology (RRCAT), Indore, India The experiment is performed using a three-dimensional double reflection geometrical set-up (Fig. 1). In the

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set-up a Cu K x-ray tube with a 3mm window is used as the parent photon source and a metallic foil of Mo is used as primary exciter. The Cu K x-rays (8.136 keV) are unable to produce K shell vacancies in Mo, therefore, bremsstrahlung radiation from the parent source is to be used for excitation of primary exciter. For each measurement, the primary exciter (active area 4.8 cm^2 each) is at a distance of 48 mm from the x-ray tube at an inclination of 45° to the incident beam. Thick circular target of Tungsten (99.9 % pure) having thickness 0.527 mg/cm^2 was on a solid support inclined at angle of 45° and at a distance of 50 mm from the Primary exciter. A Peltier cooled detector [10 mm^2, Be window thickness 0.5 µm] with FWHM ~240 eV in vertical configuration to detect the L x-rays emitted from the experimental target and to reduce the scattered background. The detector is clamped on a mount. The angle scanned by the detector is measured with respect to the direction of the electric vector of the exciting primary x-ray beam. The detector in the direction of the electric vector corresponds to 0° angle. The angle scan is from 0° to 120° at an interval of 30°. The obtained statistical uncertainty was ~5% with Mo exciter.

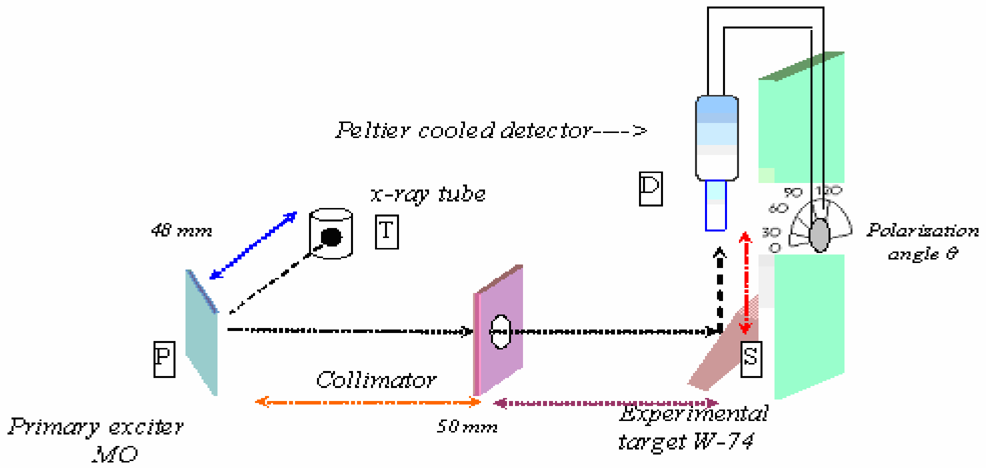

Fig. 1. Experimental set-up used for the measurements.

FORMULATION AND CALCULATION

After applying the multi-peak Gaussian fits (fig. 2) for various L x-ray peaks (ℓ, α, β and γ) depending upon their relative intensities, the collected counts are manipulated by applying various corrections. The background subtracted counts of different L x-ray peaks are normalized to time 10000 sec. at each angle. The counts collected are further corrected for solid angle correction, scattered Bremstarhlung contribution to L x-rays by subtracting the determined percentages of the counts from the counts for each L x-ray peak.

COSTER-KRONIG CORRECTION

To compare with the theoretical results, the experimental values are to be corrected for the transfer of isotropic vacancies from L1 and L2 to L3. The correction (Corr.) is counted in terms of ratio of L3 ionization probability to L3 hole production probability as;

$$Corr. = \frac{\sigma_3}{\sigma_3 + \sigma_2 f_{23} + \sigma_1 (f_{13} + f_{12} f_{23})} \quad --- \quad (1)$$

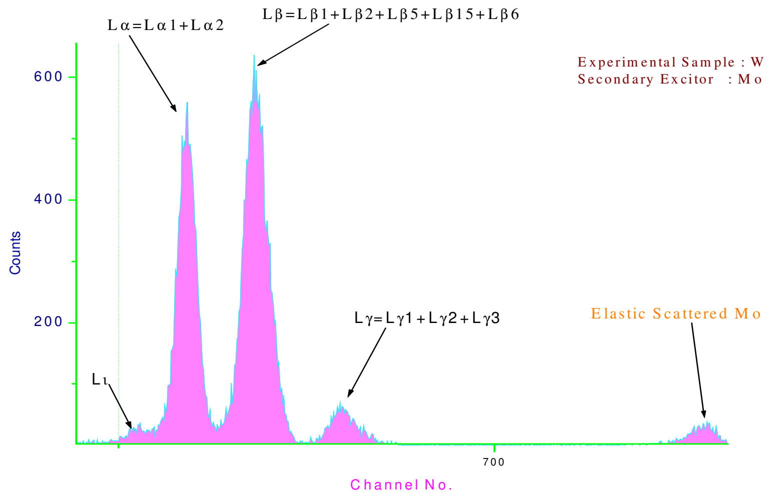

Fig. 2. Typical L x-ray spectrum with multi-peak Gaussian fits for various L x-ray peaks (ℓ, α, β and γ) depending upon their relative intensities.

where $\sigma_i^{'s}$ are sub-shell ionization cross-sections and $f_{ij}^{'s}$ are the intra sub-shell transition probabilities known as Coster-Kronig transition probabilities. For the present calculations the value of $\sigma_i^{'s}$ and $f_{ij}^{'s}$ are taken from Scofield's[5] and Krause's[6] data. The correction at Mo K x-ray energy results as = 0.81 and accordingly, the L x-ray counts for each peak at all the angles at energy 17.781 keV are corrected by applying this correction.

RESULTS AND DISCUSSION

In the recent paper of Barrea *et al.*[7], it is found that the co-ordinate system (x, y, z) in schematic diagram of present experimental set up (fig. 1) is very much similar to their dedicated instrumentation designed for an-isotropic distribution measurements. They interpreted that with incident photons oriented along z-axis and the emitted x-rays in the xy plane, the rotation of detector in xy plane with respect to x-axis is a variation of azimuth angle ϕ at a polar angle θ between incoming photon and the outgoing photon. On these guidelines, the present measurements come out to be distribution studies in the polarization plane at polar angle θ = 90°.

Therefore, the angular distribution expression becomes as[7]

$$WL_g(90°,0°)=\frac{W_0}{4\pi}\left(1+\alpha_2\left[A_{20}(-1.25)\right]\right) \qquad \text{--- (2)}$$

On the similar lines for ϕ = 30°, 60°, 90° and 120°,

$$WL_g(90°,30°)=\frac{W_0}{4\pi}\left(1+\alpha_2\left[(-0.875)A_{20}\right]\right)$$

$$WL_g(90°,60°)=\frac{W_0}{4\pi}\left(1+\alpha_2\left[(-0.125)A_{20}\right]\right)$$

$$WL_g(90°,90°)=\frac{W_0}{4\pi}\left(1+\alpha_2\left[(0.250)A_{20}\right]\right)$$

$$WL_g(90°,120°)=\frac{W_0}{4\pi}\left(1+\alpha_2\left[(-0.125)A_{20}\right]\right) \qquad \text{--- (3)}$$

Since at angle ϕ for each L_g peak, factor $W_0/4\pi$ is same and only α_2 that depends on the J values of the initial and final stages of the ionized atom has values 0.5, 0.1, -0.4 and 0.1 for L_ℓ, $L_{\alpha 1}$, $L_{\alpha 2}$ and $L_{\beta 2}$ respectively, therefore, at each azimuth angle ϕ, A_{20} are evaluated from different pairs of equations for Lg's and their average is taken. The average values at different ϕ's are listed in table (1). Excluding the departed A_{20} values[2] at ϕ=0° and 30° that is >0.5, the values at all other angles agrees within 10% error in each individual value and the weighted average of these values comes 0.243 ± 0.014. Furthermore, the experimental alignment parameter value is at 32% deviation from the value ~0.169 calculated using non-relativistic dipole approximation in a point Coulomb potential[8]. It is found that the CK correction to the L counts is 0.81 at Mo K x-ray energy but the variation in experimental alignment values with and without CK is ~1%. These quoted percentage variations in A_2 values further involve 5-7% uncertainties in parameters σ_i's and f_{ij}'s used for the evaluations of correction terms.

Table 1. Comparison of A_{20} (Experimental), and A_{20} (Theoretical) Values for W at 17.781 keV.

Energy (keV)	Azimuthal angle (ϕ)	Alignment parameter A_{20}		
		Experimental Without CK correction	Experimental With CK correction	Theoretical Using NDA
17.781	0°	0.779±0.078	0.782±0.078	~0.169
	30°	0.966±0.100	0.968±0.100	
	60°	0.252±0.025	0.252±0.025	
	90°	0.215±0.022	0.216±0.022	
	120°	0.276±0.028	0.278±0.028	

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