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Diffracted intensities from curved crystallites with layer shift. General case. By B. K. Ray, A. K. De and S. Bhattacherjee, *Department of Physics, IIT, Kharagpur* 721302, *India*

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Abstract

A general expression for the diffracted intensities from an aggregate of cylindrically curved crystallites with rotational shifts of layers by different amounts has been worked out using a model and treatments similar to those of previous work [Ray, De & Bhattacherjee (1978). *Acta Cryst.* A**34**, 637–638]. Numerical computations for several cases of layer shift showed that the heights of the diffraction peaks decrease accompanying slight changes in peak positions as the unit of angular shift decreases.

In two successive publications (Ray, De & Bhattacherjee, 1978; De, Ray & Bhattacherjee, 1979), the authors derived expressions for the diffracted intensities of X-rays from disordered curved crystallites following the model and treatments similar to those adopted by Mitra & Bhattacherjee (1971). One of the disorders considered was characterized by shifts of coaxial cylindrical layers. The shift of a layer was assumed to take place parallel to itself with rotation about the common axis with respect to its neighbouring layer by angular distances $\varphi/2$ and $\varphi/3$ analogously to the $b/2$ and $b/3$ shifts in the plane lattice layer as discussed by Wilson (1962). Wilson's approach to the case of curved crystallites can be extended and intensity expressions for the above cases readily worked out. However, it was considered necessary to derive a general expression for the diffracted intensities from disordered curved crystallites with layer shift in order to discuss the effect on the intensity as the shift changes gradually.

The present calculation is based on the same model of a disordered curved crystallite and all the symbols carry the same meaning as described in the previous work (Ray, De & Bhattacherjee, 1978; De, Ray & Bhattacherjee, 1979). Here, also, R_m and W_m are taken to be the probabilities of the mth layer being in the right and wrong places, respectively. If K is an integer and the unit angular shift is given by φ/K, then there are $(K-1)$ wrong places corresponding to the angles of shift $\rho\varphi/K$ where ρ may assume the values 1, 2, 3,..., $(K-1)$. Utilizing the conditions

$$R_m + (K-1)\,W_m = 1,$$
$$R_0 = 1, \quad W_0 = 0$$

and following Wilson (1962), we have

$$R_m = (1/K)\{1 + (K-1)[1 - K\alpha/(K-1)]^m\}$$

and

$$W_m = (1/K)\{1 - [1 - K\alpha/(K-1)]^m\},$$

where α is the probability of slip along the arc direction and φ is the angle subtended by two neighbouring lattice points on the same arc at the common axis. The average angular position of a lattice point (r, m, t) becomes $[r + (K-1)/2W_m]\varphi$ in the displaced layer. Inserting this modified value, the intensity $I(hKl_0)$ can be shown to be

$$\begin{aligned} I(hKl_0) = {} & T^2 N \sum_{m=0}^{M-1}\sum_{n=0}^{M-1} (J_0\{x_m^2 + y_n^2 \\ & - 2x_m y_n \cos[(K-1)(W_m - W_n)/2]\varphi\}^{1/2}) \\ & + T^2 \sum_{m=0}^{M-1}\sum_{n=0}^{M-1}\sum_{q=1}^{N-1} (N-q) \\ & \times (J_0\{x_m^2 + y_n^2 - 2x_m y_n \\ & \times \cos[q + (K-1)(W_m - W_n)/2]\varphi\}^{1/2} \\ & + J_0\{x_m^2 + y_n^2 - 2x_m y_n \\ & \times \cos[q + (K-1)(W_n - W_m)/2]\varphi\}^{1/2}), \end{aligned} \quad (1)$$

where

$$x_m = QN(h + mK\varphi)(1 - l_0^2/l^2)^{1/2},$$
$$y_n = QN(h + nK\varphi)(1 - l_0^2/l^2)^{1/2},$$
$$Q = 2\pi/N\varphi,\ h = (2a\sin\theta)/\lambda,\ K = 2b\sin\theta/\lambda,$$
$$l\cos\gamma = l_0 \text{ (integer)},\ sc/\lambda = l,$$

where γ is the angle between the vector s ($|s| = 2\sin\theta$) and the z axis of the coordinate system. M and N are the number of coaxial layers and the number of lattice points on each arc, respectively. a is the repeat distance between two neighbouring lattice sites on an arc on the first coaxial layer, b is the radial repeat distance of a layer and c is the repeat distance along the z direction. Introducing as before $\gamma_1 = c/a$ and $\gamma_2 = b/a$, the above equation can be written as

$$\begin{aligned} I(hKl_0) = {} & T^2 N \sum_{m=0}^{M-1}\sum_{n=0}^{M-1} J_0\{B[u_m^2 + v_n^2 - 2u_m v_n \\ & \times \cos(K-1)(W_m - W_n)\varphi/2]^{1/2}\} \\ & + T^2 \sum_{m=0}^{M-1}\sum_{n=0}^{M-1}\sum_{q=1}^{N-1} (N-q)[J_0(B\{u_m^2 + v_n^2 \\ & - 2u_m v_n \cos[q + (K-1)(W_m - W_n)/2]\varphi\}^{1/2}) \\ & + J_0(B\{u_m^2 + v_n^2 - 2u_m v_n \\ & \times \cos[q + (K-1)(W_n - W_m)/2]\varphi\}^{1/2})], \end{aligned} \quad (2)$$

where

$$B = QNh[1 - l_0^2/(r_1^2 h^2)]^{1/2},$$
$$u_m = 1 + mr_2\varphi,$$
$$v_n = 1 + nr_2\varphi.$$

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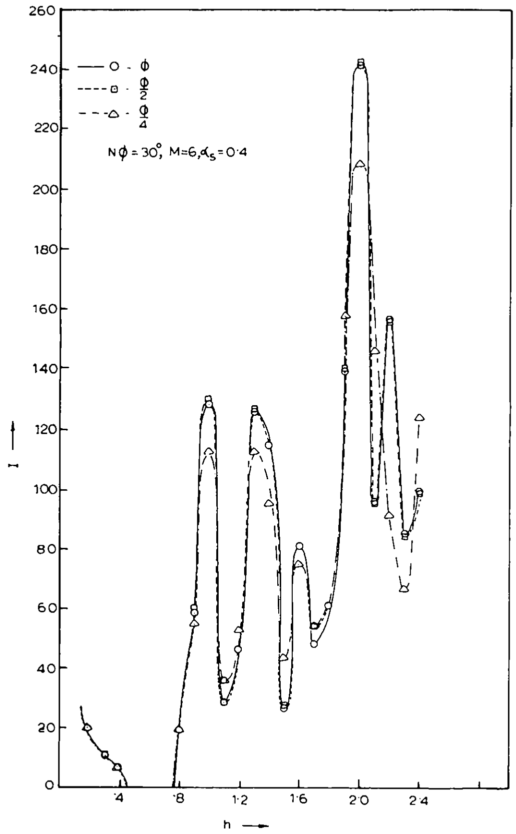

Fig. 1. Diffracted intensities from a cluster of cylindrical crystallites with faults $\varphi/2$ and $\varphi/4$ and without fault.

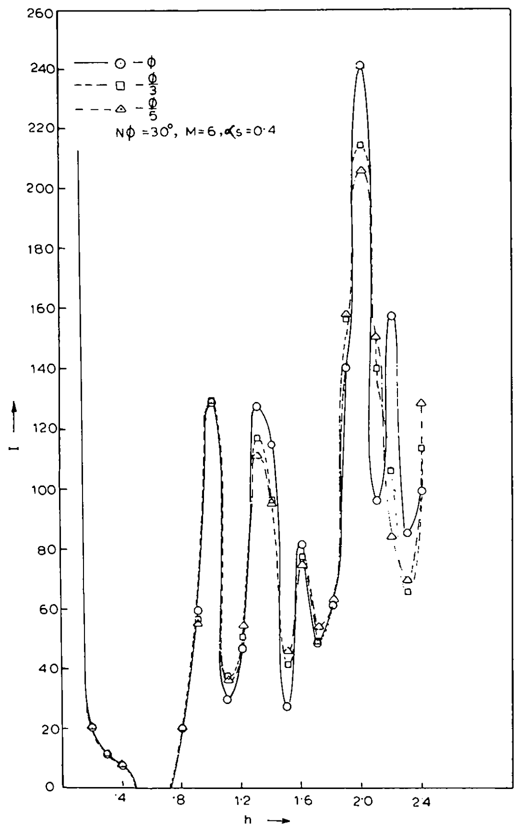

Fig. 2. Diffracted intensities from a cluster of cylindrical crystallites with faults $\varphi/3$ and $\varphi/5$ and without fault.

Equation (2) is the general expression for the diffracted intensities by an agglomerate composed of fragments of cylindrically curved crystallites with layer shifts. Substitution of different values of K in (2) leads to the intensity expressions for different cases of layer shift. For $K = 2$ and 3, it reduces to equation (2) of Ray, De & Bhattacherjee (1978) and equation (2) of De, Ray & Bhattacherjee (1979) corresponding to the $\varphi/2$ and $\varphi/3$ shifts, respectively. Based on this general expression, numerical computations have been carried out for intensities with different values of K corresponding to different values of unit angular shifts. Figs. 1 and 2 show the results of the numerical calculations for $K = 2$, 4 and 3, 5 corresponding to the unit layer shifts $\varphi/2$, $\varphi/4$ and $\varphi/3$, $\varphi/5$, respectively. The intensity distribution for the crystallite without faults is also shown for comparison.

Although the broad features of the patterns are almost similar in all the cases, it is noted that the peak height decreases, accompanying slight changes in peak positions, as the unit angular shift decreases. It may be thus concluded that the main effect of layer shift appears as a decrease in the relative peak height as the value of the unit angular shift decreases.

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