X-ray diffraction from disordered cylindrical lattices.

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Expressions for the diffracted intensities from an aggregate of cylindrically curved crystallites with disordered lattices have been worked out. The treatment is very much similar to that of Mitra & Bhattacherjee [*Acta Cryst.* (1971), A**27**, 22–28]. The lattice disorders considered consist of layer shift and variability of interlayer spacings. Results of numerical computations have been discussed and compared with those of cylindrical crystallites without faults.

In a series of publications, Mitra (1965), Mitra & Bhattacherjee (1968, 1971) and Nigam, Mukherjee & Bhattacherjee (1976) developed an elementary theory of X-ray diffraction by curved crystallites and derived expressions for diffracted intensities from conglomerates of cylindrically curved crystallites of various models without any simplifying assumptions. The intensity expressions are very simple and are quite suitable for numerical computations. Mitra & Bhattacherjee (1975) applied their theory to the X-ray line profiles of halloysites and on the basis of their results concluded a satisfactory model of a cylindrical lattice for metahalloysites.

Following the model and treatments developed by these authors, we have in the present study attempted to derive expressions for diffraction intensities from cylindrical lattices with two different types of stacking faults which are of common occurrence in many types of layered structure, especially in silicate minerals.

The two specific stacking disorders considered are one characterized by the layer shift and one characterized by variability of interlayer spacings in layer lattices, both as discussed and studied by Mitra & Bhattacherjee (1969, 1970). The basic model is exactly similar to that of Mitra & Bhattacherjee (1971, Fig. 1*a,b*) with the cylindrical layers displaced relative to one another. All the symbols used in this work carry the same meaning as defined by these authors.

Layer shift characterizing the first type of disorder consists of a coaxial cylindrical layer displaced parallel to itself with respect to its adjacent layer by an angular distance $\varphi/2$ about the common axis of the crystallites. If there is a chance of the mth layer sliding by an angular distance $\varphi/2$, then the average angular position of the lattice point (r,m,t) on the displaced layer with respect to the undisturbed one is given by $(r + W_m/2)\varphi$ where W_m and R_m are the probabilities that the mth layer is in the wrong and right place, respectively, as defined by Wilson (1962). Replacing the azimuthal coordinate $r\varphi$ by $(r + W_m/2)\varphi$ and following the same procedure as that of Mitra & Bhattacherjee (1971), the average intensity $I(s)$ from an assembly of disordered crystallites is found to be given by

$$I(s) = T^2 \sum_{m=0}^{M-1} \sum_{n=0}^{M-1} \sum_{p=-\infty}^{+\infty} \left\{ J_p \frac{2\pi s}{\lambda} \left[1 - \frac{l_0^2}{l^2} \right]^{1/2} (R + mb) \right\}$$

$$\times J_p \left\{ 2\pi \frac{1}{N\varphi} N \left(1 - \frac{l_0^2}{l^2} \right)^{1/2} \left(\frac{R\varphi s}{\lambda} + \frac{nb\varphi s}{\lambda} \right) \right\}$$

$$\times \frac{\sin^2(np\varphi)/2}{\sin^2(p\varphi)/2} \exp\left[ip(W_m - W_n) \frac{\varphi}{2} \right]. \quad (1)$$

Proceeding as Mitra & Bhattacherjee (1971), $I(hkl_0)$ can be written as

$$I(hkl_0) = T^2 N \sum_{m=0}^{M-1} \sum_{n=0}^{M-1} J_0 \left[x^2 + y^2 - 2xy \cos(W_m - W_n)\frac{\varphi}{2} \right]^{1/2}$$

$$+ T^2 \sum_{m=0}^{M-1} \sum_{n=0}^{M-1} \sum_{q=1}^{N-1} (N - q)$$

$$\times \left\{ J_0 \left[x^2 + y^2 - 2xy \cos(2q + W_m - W_n)\frac{\varphi}{2} \right]^{1/2} \right.$$

$$\left. + J_0 \left[x^2 + y^2 - 2xy \cos(2q - W_m - W_n)\frac{\varphi}{2} \right]^{1/2} \right\} \quad (2)$$

where $x = QN(h + mk\varphi)[1 - (l_0^2/l^2)]^{1/2}$, $y = QN(h + nk\varphi)[1 - (l_0^2/l^2)]^{1/2}$, T = total number of layers in the z direction stacked at an interval c, R = radius of the first coaxial cylindrical layer, $l = sc/\lambda$; l_0 (an integer) = $(sc \cos \gamma)/\lambda$ where γ is the angle between the s and z directions, m,n = number indicating the position of a layer on which a particular lattice point is located, $h = (2a \sin \theta)/\lambda$, $k = (2b \sin \theta)/\lambda$, q = an
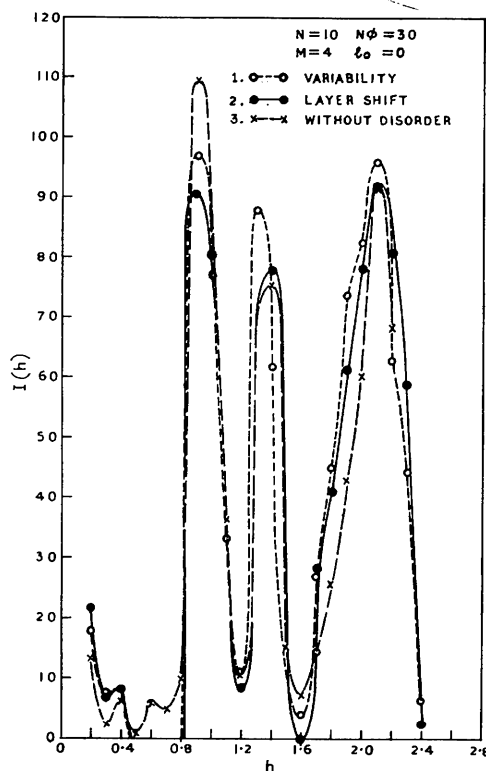

Fig. 1. Intensities from an axially parallel aggregate of cylindrical fragments with (1 and 2) and without (3) disorder.

integer, M = total number of cylindrical layers, N = total number of atoms in each arc.

The second type of stacking is characterized by variability of interlayer spacings having a structure similar to that discussed by Wilson (1962) and studied by Mitra & Bhattacherjee (1969). In this defect model the interlayer distance between successive cylindrical layers will be the radial repeat distance b. If g is the mean fractional change in the interlayer distance in the b direction and α_c is the probability of such change taking place, then replacing b by $b(1 + g\alpha_c)$, equation (2) can be written when both the faults are present as

$$
\begin{aligned}
I(hkl_0) &= T^2 N \sum_{m=0}^{M-1} \sum_{n=0}^{M-1} J_0 \left[QNh \left(1 - \frac{l_0^2}{r_1^2 h^2}\right)^{1/2} \right. \\
&\times \left\{ [1 + mr_2(1 + g\alpha_c)\varphi]^2 + [1 + nr_2(1 + g\alpha_c)\varphi]^2 \right. \\
&- 2[1 + mr_2(1 + g\alpha_c)\varphi][1 + nr_2(1 + g\alpha_c)\varphi] \\
&\times \left. \left. \cos(W_m - W_n)\varphi/2\right\}^{1/2} \right] \\
&+ T^2 \sum_{m=0}^{M-1} \sum_{n=0}^{M=1} \sum_{q=1}^{N-1} (N-q) \left[J_0 \left(QNh \left(1 - \frac{l_0^2}{r_1^2 h^2}\right)^{1/2} \right) \right. \\
&\times \left\{ [1 + mr_2(1 + g\alpha_c)\varphi]^2 + [1 + nr_2(1 + g\alpha_c)\varphi]^2 \right. \\
&- 2[1 + mr_2(1 + g\alpha_c)\varphi][1 + nr_2(1 + g\alpha_c)\varphi] \\
&\times \left. \left. \cos(2q + W_m - W_n)\varphi/2 \right\}^{1/2} \right) \\
&+ J_0 \left(QNh \left(1 - \frac{l_0^2}{r_1^2 h^2}\right)^{1/2} \{[1 + mr_2(1 + g\alpha_c)\varphi]^2 \right. \\
&+ [1 + nr_2(1 + g\alpha_c)\varphi]^2 \\
&- 2[1 + mr_2(1 + g\alpha_c)\varphi][1 + nr_2(1 + g\alpha_c)\varphi] \\
&\times \left. \left. \cos(2q - W_m + W_n)\varphi/2 \right\}^{1/2} \right) \right]
\end{aligned}
$$

(3)

where $r_1 = c/a$ and $r_2 = b/a$.

Equation (3) reduces to equation (16) of Mitra & Bhattacherjee (1971) when $W_m = W_n = 0$ and $g = 0$ as expected. Numerical computations for typical cases have been carried out. Fig. 1 illustrates the general pattern of the curves for three cases. Results of the calculations have also been compared with those of Bhattacherjee & Mathur (1974) and Mitra & Bhattacherjee (1971) for cylindrical crystallites without defects. It is observed that the general pattern is more or less of the same form in the three cases, although comparison of curves 1, 2 and 3 suggests that the relative heights vary with the order of the peak. The heights of the second and third-order peaks of curves 1 and 2, particularly 1, appear to have increased compared with that of curve 3. A more detailed study of the change due to the variation of parameters in the intensity pattern is in progress.

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The structural classification of crystal point symmetries: *corrigenda et addendum.* By J. D. H. DONNAY,

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In *Internationale Tabellen zur Bestimmung der Kristallstrukturen (IT)* [Vol. I. (1935), Berlin: Borntraeger] Carl Hermann followed the Mallard classification into crystal systems. The 'trigonal system' did not enter the *IT* until 1952 – a step backwards.

In the paper that appeared under the above title (Donnay, 1977), please note the following alterations: p. 979, Abstract, line 1: instead of 1935, read 1952; p. 984, References, Friedel (1926), Reprinted: instead of 1974, read 1964; p. 982, *Historical perspective*, after the first paragraph, insert the following *addendum*.

It is noteworthy that Carl Hermann (1898–1961) closely follows Mallard (1879) in his classification into systems, which appears in chapter III of *IT* (1935, pp. 49–63, particularly pp. 54–60). The resulting listing thus agrees with that advocated in this paper (Table 1, column 2) with a single exception: the orthorhombic antihemihedry C_{2v} is given in