The effect of preferred orientation on the intensity distribution of (hk) interferences*.

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The paper deals with the X-ray scattering produced by a distribution of two-dimensional lattices with preferred orientation, a problem which arises in the study of anisotropic structures of non-graphitic carbons. The problem has been treated by Guentert and Cvikevich (1964) for a special case of the orientation function ($|\cos^n\varphi|$) and a unique direction in reciprocal space (perpendicular to the axis of cylindrical symmetry of preferred orientation). The purpose of this paper is to give a general treatment of the problem.

A rigorous treatment is given for infinite and perfect lattices. The results of this treatment show that the intensity distribution of a (hk) interference can be written in the form

$$I(s,\varphi) = \frac{1}{2\pi s\sqrt{s^2 - s_h^2}} \cdot F\left(\frac{s}{s_h}, \varphi\right)$$

where s and φ are the polar coordinates of the reciprocal space vector in a system of cylindrical symmetry, s_h is the distance of the reciprocal lattice point h (=hk) from the origin. The first factor on the right-hand side is the profile of a (hk)-line for the isotropic case (von Laue, 1932). The second factor (F) contains the effect of the preferred orientation.

In the general case, F is given in a closed form by

$$F\left(\frac{s}{s_h}, \varphi\right) = 2\int_0^{\pi} g(\beta)\, d\eta$$

where g is the orientation function (the distribution of layer normals) as obtained from a study of the (001) lines and

$$\cos\beta = \cos\varphi\cos\sigma + \sin\varphi\sin\sigma\cos\eta,$$

$$\sin\sigma = \frac{s}{s_h}$$

An analytical expression for F can be given if g can be represented by a Poisson kernel, a form which is valid in many practical cases. Furthermore, the complete analytical expression for g in the form of $|\cos^n\varphi|$ for arbitrary directions in reciprocal space is given. A method to compute F from the Fourier coefficients of g has also been developed.

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Approximate solutions of the problem for finite and imperfect lattices are given as well as for structures with partial positional correlations.

As an example of the application the observed intensity distributions of (hk) interferences of a highly oriented carbon fiber are compared with calculated intensity distributions.

References :

O. J. Guentert and S. Cvikevich (1964) Carbon 1, 309.

von Laue, M. (1932) Z. Kristallogr. 82, 127.