(1965), based on a lattice-dynamical analysis of their measured phonon dispersion relations. On the whole, there is reasonably good agreement between observation and theory. The theory neglects anharmonic contributions to the Debye–Waller factors, and this could account for the observed displacements for U exceeding the calculated displacements, especially at high temperatures.

Conclusions

The data of Willis (1963) have been re-analysed with a structure-factor equation including third cumulants. The only non-vanishing third cumulant for UO_2 is c_{123} for the O atom. Introducing c^0_{123} into the analysis accounts for anisotropic anharmonic thermal motion of the O atom. c^0_{123}, B_U and B_O have been derived over the temperature range 293 to 1373 K. The e.s.d.'s of c^0_{123} are too large to allow a rigorous check of the theoretical dependence on temperature, but B_U and B_O are in reasonable agreement with those predicted by the theory of lattice dynamics.

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X-ray Diffraction from Faulted Close-Packed Structures. Analytic Solution for Integrated Intensities

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Abstract

Analytic expressions for the integrated intensities of reflexions from faulted close-packed structures have been obtained. These involve a single root of the characteristic equation (the root which corresponds to the reflexion under consideration), its coefficients and the initial conditions. The particular utility of the solution for cases where one or more roots of the characteristic equation have unit modulus is demonstrated.

Introduction

Diffraction from close-packed crystals with stacking faults has been investigated by a large number of workers and has been reviewed by Warren (1959, 1969), Wilson (1962), Cohen & Hilliard (1966) and Anantharaman, Rama Rao & Lele (1972) among others. In their pioneering papers, Wilson (1942) and Hendricks & Teller (1942) developed distinct approaches to a solution of this problem. The present paper describes a simplification in the procedure for the evaluation of integrated intensities following the difference-equation method of Wilson (1942). This method also enables an analytical solution for the diffuse diffracted intensity when the characteristic equation found from the difference equation has roots with unit modulus.

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Formulation of the problem

In general, the diffracted intensity from a possibly faulted crystal is given by (Warren, 1959)

$$I(h_3) = \psi^2 \sum_m \langle \exp [i\Phi_m] \rangle \exp (2\pi imh_3/n), \quad (1)$$

where h_1, h_2, h_3 are continuous variables in reciprocal space, ψ^2 is a function of $h_1 h_2$ which vanishes except when $h_1 = H$, $h_2 = K$, H and K being hexagonal indices with integer values, and Φ_m, the phase difference across a pair of layers m layers apart, is given by

$$\Phi_m = (2\pi/3)(H-K)\,q_m, \quad (2)$$

q_m being the displacement of the m layer from the origin layer in units of the stacking offset vector $(1/3)\langle 1100\rangle$, and n is the number of layers in the hexagonal unit cell. Thus, reflexions with $H-K=0 \pmod 3$ are unaffected by faulting.

The evaluation of the diffracted intensity, therefore, reduces to the determination of

$$J_m \equiv \langle \exp[i\Phi_m]\rangle \qquad (3)$$

for reflexions with $H-K\neq 0 \pmod 3$ and is based on the statistical specification of the distribution of stacking faults. Denoting the probability of obtaining the phase difference Φ_m across m layers by $P(\Phi_m)$, we can write

$$J_m = \sum P(\Phi_m)\exp[i\Phi_m], \qquad (4)$$

where the summation extends over all possible values of Φ_m. The probability $P(\Phi_m)$ is itself a function of the stacking-fault probability α. Once the structure and the fault are specified, the probabilities of transition from the $(m-1)$ layer to the m layer can be expressed in the form of trees from which difference equations for $P(\Phi_m)$ and consequently J_m can be found (Lele, 1974). The latter can be expressed, in general, as follows:

$$J_{m+n} + a_{n-1}J_{m+n-1} + \ldots + a_1 J_{m+1} + a_0 J_m = 0. \qquad (5)$$

A solution for this difference equation is of the form

$$J_m = C\rho^m. \qquad (6)$$

On inserting this solution in the difference equation (5) for J_m, an n-degree equation in ρ, usually called the characteristic equation, is obtained. The general solution for J_m is obtained by forming a linear combination from all the n roots, ρ_j ($j=0$ to $n-1$), of the characteristic equation. Thus,

$$J_m = \sum_{j=0}^{n-1} C_j\rho_j^m. \qquad (7)$$

The proportionality factors ($C_j, j=0$ to $n-1$) can be evaluated by first directly determining J_m ($m=0$ to $n-1$), which specify the initial conditions, and subsequently solving n simultaneous equations of the type of (7) since the roots, ρ_j, of the characteristic equation are known. Both ρ_j and C_j are generally complex and can be expressed in terms of real quantities Z_j (real as well as positive), X_j, A_j and B_j as follows:

$$\rho_j = Z_j\exp(-2\pi i X_j/n), \qquad (8)$$

$$C_j = A_j + iB_j. \qquad (9)$$

The diffracted intensity can then be obtained by substituting from (3) and (7) into (1).

$$I(h_3) = \psi^2\sum_{j=0}^{n-1}\sum_{m=-\infty}^{\infty} C_j\rho_j^{|m|}\exp(2\pi imh_3/n), \quad H-K\neq 0 \pmod 3. \qquad (10)$$

Each of the n series over m on the right-hand side of (10) is a geometric series which can be summed for $|\rho_j| < 1$ but not for $|\rho_j|=1$. Thus roots with unit modulus need to be distinguished. Let the p roots, $\rho_j, j=(n-p)$ to $(n-1)$, have unit modulus. Separating the series in (10) into two parts according as $|\rho_j|<1$ and $|\rho_j| = Z_j = 1$, we have

$$I(h_3) = \psi^2\sum_{j=0}^{n-p-1}\sum_{m=-\infty}^{\infty} C_j\rho_j^{|m|}\exp(2\pi imh_3/n) + \psi^2\sum_{j=n-p}^{n-1}\sum_{m=-\infty}^{\infty} C_j\exp(-2\pi i|m|X_j/n) \times \exp(2\pi imh_3/n),\ H-K\neq 0 \pmod 3). \qquad (11)$$

We consider the two terms on the right-hand side of (11) separately by introducing

$$I_d(h_3) = \psi^2\sum_{j=0}^{n-p-1}\sum_{m=-\infty}^{\infty} C_j\rho_j^{|m|}\exp(2\pi imh_3/n), \quad |\rho_j|<1, \qquad (12)$$

$$I_s(h_3) = \psi^2\sum_{j=n-p}^{n-1}\sum_{m=-\infty}^{\infty} C_j\exp(2\pi im/n)(h_3-X_j), \quad |\rho_j|=1. \qquad (13)$$

Summing the series over m in (12) separately for $m=1$ to ∞ and $m=-1$ to $-\infty$, we have

$$I_d(h_3) = \psi^2\sum_{j=0}^{n-p-1}\left\{A_j + \frac{C_j\rho_j}{E-\rho_j} + \frac{C_j^*\rho_j^*}{E^*-\rho_j^*}\right\}, \quad |\rho_j|<1, \qquad (14)$$

where

$$E = \exp(-2\pi ih_3/n). \qquad (15)$$

On simplification, we obtain

$$I_d(h_3) = \psi^2\sum_{j=0}^{n-p-1}[A_j(1-Z_j^2) - 2B_jZ_j \times \sin(2\pi/n)(h_3-X_j)]/[1+Z_j^2-2Z_j \times \cos(2\pi/n)(h_3-X_j)], \quad |\rho_j|<1. \qquad (16)$$

Thus, each of the $(n-p)$ roots with modulus less than unity gives rise to a *diffuse* peak at $h_3=X_j$, $j=0$ to $(n-p-1)$.

As already mentioned, the series over m in (13) cannot be summed. Usually for $|\rho_j|=1$, $B_j=0$ and X_j is an integer and (13) reduces to

$$I_s(h_3) = \psi^2\sum_{j=n-p}^{n-1}\sum_{m=-\infty}^{\infty} A_j\cos(2\pi m/n)(h_3-X_j), \quad |\rho_j|=1. \qquad (17)$$

Thus each of the p roots with unit modulus gives rise to an infinitely *sharp* peak at $h_3 = X_j$, $j = (n-p)$ to $(n-1)$.

The integrated intensity for each of the n reflexions corresponding to the n roots of ρ can be obtained by separately integrating each term in (16) and (17) over h_3 from $-n/2$ to $+n/2$ and can be shown to be equal to A_j apart from a constant.

The solution for the C_j can be effected by applying Cramer's rule to equations of the type of (7) and we shall be concerned in the next section of this paper with a simplification in their evaluation so that each C_j can be expressed in terms of a single root, namely the corresponding root ρ_j, the coefficients of the characteristic equation and the initial conditions.

By carrying out the summation in (14), and replacing the elementary symmetric functions of ρ_j by a_j and the expressions involving C_j by J_m, Gevers (1954; see also Holloway, 1969*a*) has obtained an expression for the diffracted intensity that involves only a_j and J_m and thus does not necessitate a solution of the characteristic equation nor of the simultaneous equations for C_j. Obviously, this solution is not valid when one or more roots, *i.e.* ρ_j, have a modulus equal to unity. Examples of such a situation are provided by the triple fault in f.c.c. structures (Sato, 1966) and the extrinsic or layer displacement fault in h.c.p. structures (Lele, Anantharaman & Johnson, 1967; Pandey, Lele & Krishna, 1980).

We shall also consider, with applications, in the last section of this paper, the special utility of the present method of evaluating C_j in obtaining the diffracted intensity when one or more of the ρ_j have unit modulus.

Integrated intensities

Substituting from (6) into (5) and simplifying, we get a characteristic equation of the following general form

$$F(\rho) \equiv \rho^n + a_{n-1}\rho^{n-1} + \ldots + a_1\rho + a_0 = 0. \quad (18)$$

In terms of its roots, this can be expressed as

$$F(\rho) = (\rho - \rho_0)(\rho - \rho_1)\ldots(\rho - \rho_{n-2})(\rho - \rho_{n-1}) = 0. \quad (19)$$

The coefficients, a_j, and the roots, ρ_j, $j = 0$ to $(n-1)$ are functions of the fault probability and are related through standard expressions.

From (7), we have

$$\begin{aligned} C_0\rho_0^{n-1} + C_1\rho_1^{n-1} + \ldots + C_{n-2}\rho_{n-2}^{n-1} + C_{n-1}\rho_{n-1}^{n-1} &= J_{n-1} \\ C_0\rho_0^{n-2} + C_1\rho_1^{n-2} + \ldots + C_{n-2}\rho_{n-2}^{n-2} + C_{n-1}\rho_{n-1}^{n-2} &= J_{n-2} \\ \vdots \qquad \vdots \qquad & \\ C_0\rho_0 + C_1\rho_1 + \ldots + C_{n-2}\rho_{n-2} + C_{n-1}\rho_{n-1} &= J_1 \\ C_0 + C_1 + \ldots + C_{n-2} + C_{n-1} &= J_0. \end{aligned} \quad (20)$$

Using Cramer's rule, we have from (20)

$$C_j = N_j/D, \quad j = 0 \text{ to } (n-1), \quad (21)$$

where N_j and D represent the following determinants:

$$N_j = \begin{vmatrix} \rho_0^{n-1} & \rho_1^{n-1}\ldots\rho_{j-1}^{n-1} & J_{n-1} & \rho_{j+1}^{n-1}\ldots\rho_{n-2}^{n-1} & \rho_{n-1}^{n-1} \\ \rho_0^{n-2} & \rho_1^{n-2}\ldots\rho_{j-1}^{n-2} & J_{n-2} & \rho_{j+1}^{n-2}\ldots\rho_{n-2}^{n-2} & \rho_{n-1}^{n-2} \\ \vdots & \vdots \quad \vdots & \vdots & \vdots \quad \vdots & \vdots \\ \rho_0 & \rho_1 \ldots \rho_{j-1} & J_1 & \rho_{j+1}\ldots\rho_{n-2} & \rho_{n-1} \\ 1 & 1 \ldots 1 & J_0 & 1 \ldots 1 & 1 \end{vmatrix},$$

$$j = 1 \text{ to } (n-1); \quad (22)$$

$$D = \begin{vmatrix} \rho_0^{n-1} & \rho_1^{n-1}\ldots\rho_{n-2}^{n-1} & \rho_{n-1}^{n-1} \\ \rho_0^{n-2} & \rho_1^{n-2}\ldots\rho_{n-2}^{n-2} & \rho_{n-1}^{n-2} \\ \vdots & \vdots \quad \vdots & \vdots \\ \rho_0 & \rho_1 \ldots \rho_{n-2} & \rho_{n-1} \\ 1 & 1 \ldots 1 & 1 \end{vmatrix}. \quad (23)$$

We shall consider a further simplification for the specific case of C_0. The determinant N_0 vanishes when $\rho_j = \rho_k (k > j \neq 0)$, since it then has two columns identical. Hence, by the remainder theorem, it has factors $(\rho_j - \rho_k)$ where $k > j \neq 0$. We may thus write

$$\begin{aligned} N_0 = (\rho_1 - \rho_2)(\rho_1 - \rho_3)\ldots(\rho_{n-3} - \rho_{n-1}) \\ \times (\rho_{n-2} - \rho_{n-1}) M_0 = P_0 M_0, \end{aligned} \quad (24)$$

say, where M_0 has to be determined. By a similar argument, D has factors $(\rho_j - \rho_k)$ with $k > j \neq 0$ as also factors $(\rho_0 - \rho_k)$ with $k \neq 0$. Hence,

$$D = P_0(\rho_0 - \rho_1)(\rho_0 - \rho_2)\ldots(\rho_0 - \rho_{n-2})(\rho_0 - \rho_{n-1})\,D', \quad (25)$$

where D' has to be evaluated. To do this, we observe that D is a homogeneous polynomial of degree $n(n-1)/2$ in ρ_j and thus D' must be independent of them and so is a numerical constant which can be shown to be unity. Thus

$$\begin{aligned} D &= P_0(\rho_0 - \rho_1)(\rho_0 - \rho_2)\ldots(\rho_0 - \rho_{n-2})(\rho_0 - \rho_{n-1}) \\ &= P_0 E_0, \end{aligned} \quad (26)$$

say. The $(n-1)(n-2)/2$ factors representing P_0 are common to N_0 and D and will cancel on substitution in (21). Therefore, only the last $(n-1)$ factors need further consideration. Let us introduce the coefficients b_j, $j = 0$ to $(n-2)$ through

$$\begin{aligned} F(\rho)/(\rho - \rho_0) \equiv (\rho - \rho_1)(\rho - \rho_2)\ldots(\rho - \rho_{n-2}) \\ \times (\rho - \rho_{n-1}) = \rho^{n-1} + b_{n-2}\rho^{n-2} \\ + \ldots + b_1\rho + b_0. \end{aligned} \quad (27)$$

From (26) and (27), we have

$$E_0 = D/P_0 = \rho_0^{n-1} + b_{n-2}\rho_0^{n-2} + \ldots + b_1\rho_0 + b_0. \quad (28)$$

Considering the expansion of D in terms of the elements of the first column of D and their cofactors (equation 23), it is obvious that the b_j are just the cofactors except for the common factor P_0. A similar expansion of N_0 (equation 22) thus gives

$$M_0 = N_0/P_0 = J_{n-1} + b_{n-2}J_{n-2} + \ldots + b_1J_1 + b_0J_0. \quad (29)$$

Substituting in (21) from (28) and (29), we have

$$C_0 = [J_{n-1} + b_{n-2}J_{n-2} + \ldots + b_1J_1 + b_0J_0] \times [\rho_0^{n-1} + b_{n-2}\rho_0^{n-2} + \ldots + b_1\rho_0 + b_0]^{-1}. \quad (30)$$

An alternative expression for C_0 in terms of a_j rather than b_j can be obtained by multiplying (27) by $(\rho - \rho_0)$ on both sides, substituting for $F(\rho)$ from (18) and equating the coefficients of ρ^j ($j = 1$ to $n - 1$) on both sides. Thus,

$$b_{j-1} - b_j\rho_0 = a_j, \qquad j = 1 \text{ to } (n-1). \quad (31)$$

The solution of this difference equation is

$$b_j = \rho_0^{n-j-1} + a_{n-1}\rho_0^{n-j-2} + \ldots + a_{j+2}\rho_0 + a_{j+1}. \quad (32)$$

Substituting from the above into (30), we obtain, after rearranging in decreasing powers of ρ_0,

$$\begin{aligned} C_o = {} & [J_0\rho_0^{n-1} + (J_0a_{n-1} + J_1)\rho_0^{n-2} + \ldots \\ & + (J_0a_2 + J_1a_3 + \ldots + J_{n-3}a_{n-1} + J_{n-2})\rho_0 \\ & + (J_0a_1 + J_1a_2 + \ldots + J_{n-2}a_{n-1} + J_{n-1})] \\ & \times [n\rho_0^{n-1} + (n-1)a_{n-1}\rho_0^{n-2} \\ & + \ldots + 2a_2\rho_0 + a_1]^{-1}. \end{aligned} \quad (33)$$

Since the analytical solutions (equations 30 and 33) for C_0 involve only the corresponding root of the characteristic equation, namely ρ_0, apart from the coefficients (a_j or b_j) and the initial conditions, it follows that knowledge of the value of a single root, ρ_j, is sufficient for the evaluation of the respective C_j. On the other hand, a direct evaluation of C_j from (21) requires a knowledge of all the roots rather than the coefficients of the characteristic equation. Since expressions for the coefficients are generally much simpler than those for the roots (in fact for equations of degree higher than four, it may not be possible at all to have analytical expressions for the roots), the convenience in obtaining the integrated intensity from (33) is obvious.

Applications for cases with solutions having unit modulus

The diffracted intensity from diffuse reflexions can be obtained by summing the series on the right-hand side of (14) following the procedure of Gevers (1954) and Holloway (1969*a*). Consequently, elementary symmetric functions of only those roots with $|\rho_j| < 1$ will appear in this expression. These can be obtained by dividing (18) by p factors $(\rho - \rho_j)$, $|\rho_j| = 1, j = (n-p)$ to $(n-1)$, giving

$$G(\rho) \equiv \rho^{n-p} + d_{n-p-1}\rho^{n-p-1} + \ldots + d_1\rho + d_0 = 0. \quad (34)$$

The roots of this equation are identical to those involved in the summation mentioned above and hence the elementary symmetric functions of these roots are equal to the d_j, apart from their signs. Thus a_j should be replaced by d_j in the analytic solution for the diffracted intensity obtained by Gevers and Holloway. In a similar fashion, the J_m (equation 7), which correspond to a sum over all roots, should be replaced by K_m which have a sum over the roots with $|\rho_j| < 1$ only. Thus,

$$K_m = \sum_{j=0}^{n-p-1} C_j\rho_j^m. \quad (35)$$

Utilizing (7), we can rewrite (35) as

$$K_m = J_m - \sum_{j=n-p}^{n-1} C_j\rho_j^m. \quad (36)$$

We have thus obtained a self-consistent set consisting of the characteristic equation (34) and the initial conditions (equation 36) which no longer have the effects of any roots with unit modulus and thus can be used as input for the calculation of the diffracted intensity by the method of Gevers (1954). As already mentioned, the diffracted intensity corresponding to the roots with unit modulus consists of sharp peaks and has to be superposed on the diffuse intensity corresponding to the roots with non-unit modulus.

As an illustration of this procedure, we shall consider the case of extrinsic faulting in h.c.p. crystals. Following Holloway (1969*b*), the characteristic equation is

$$\rho^4 - (1-\alpha)^2\rho^2 - 2\alpha(1-\alpha)\rho - \alpha^2 = 0, \quad (37)$$

which has one root, say ρ_3 with unit modulus ($Z_3 = 1$; $X_3 = 0$), while the initial conditions are

$$\begin{aligned} & J_0 = 1, \quad J_2 = (2 - 7\alpha + 6\alpha^2)/2(1+\alpha), \\ & J_1 = -1/2, J_3 = (-1 + 5\alpha - 3\alpha^2 - 3\alpha^3)/2(1+\alpha). \end{aligned} \quad (38)$$

Dividing (37) by $(\rho - \rho_3) \equiv (\rho - 1)$, we have

$$\rho^3 + \rho^2 + (2\alpha - \alpha^2)\rho + \alpha^2 = 0. \quad (39)$$

Thus,

$$b_2 = 1, b_1 = 2\alpha - \alpha^2, b_0 = \alpha^2. \quad (40)$$

Utilizing (38) and (40), we obtain from (30)

$$\begin{aligned} C_3 & = \frac{J_3 + J_2b_2 + J_1b_1 + J_0b_0}{\rho_3^3 + b_2\rho_3^2 + b_1\rho_3 + b_0} \\ & = (1-2\alpha)^2/4(1+\alpha)^2. \end{aligned} \quad (41)$$

From (36), (38) and (41), we get

$$K_0 = 3(1 + 4\alpha)/4(1 + \alpha)^2,$$
$$K_1 = -3(1 + 2\alpha^2)/4(1 + \alpha)^2,$$
$$K_2 = 3(1 - 2\alpha)(1 - 2\alpha^2)/4(1 + \alpha)^2. \quad (42)$$

Following Gevers (1954) and Holloway (1969*a*), the diffracted intensity for the diffuse reflexions is given by

$$I_d(h_3) = K_0 + \left[2 \sum_{j=0}^{3} A_j \cos(\pi j h_3) \Big/ \sum_{j=0}^{3} B_j \cos(\pi j h_3)\right], \quad (43)$$

where

$$\begin{aligned} A_0 &= b_2 K_1 + b_1(K_2 + b_2 K_1) - b_0^2 K_0, \\ A_1 &= (1 + b_1)K_1 + (b_2 + b_0)(K_2 + b_2 K_1) - b_1 b_0 K_0, \\ A_2 &= b_0 K_1 + K_2 + b_2 K_1 - b_2 b_0 K_0, \\ A_3 &= -b_0 K_0, \\ B_0 &= 1 + b_2^2 + b_1^2 + b_0^2, \\ B_1 &= 2(b_2 + b_2 b_1 + b_1 b_0), \\ B_2 &= 2(b_1 + b_2 b_0), \\ B_3 &= 2b_0. \end{aligned} \quad (44)$$

Substituting from (40), (42) and (44) in (43), we have after simplification

$$\begin{aligned} I_d(h_3) = \{&3\alpha(1 - \alpha)[2 - 3\alpha + 2\alpha^2 + (1 + \alpha - 2\alpha^2) \\ &\times \cos \pi h_3 + 2\alpha \cos^2 \pi h_3]\}/\{2(1 + \alpha) \\ &\times [1 + \alpha^2 + 2\alpha \cos \pi h_3] \\ &\times [(1 - \alpha)^2 + (1 - \alpha^2) \\ &\times \cos \pi h_3 + 2\alpha \cos^2 \pi h_3]\}, \end{aligned} \quad (45)$$

which is identical with the expression obtained by Lele, Anantharaman & Johnson (1967) and Holloway (1969*b*). It may be noted that except for the root with unit modulus and the corresponding integrated intensity, which could be obtained very simply, no other root or integrated-intensity values were necessary for the calculations.

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The Fragile Lattice Packings of Spheres in Four-Dimensional Space

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Abstract

In a fragile packing of spheres, the density of the packed spheres is minimized. There are exactly nine distinct indecomposable fragile lattice packings in four-dimensional space; they are described in terms of their associated quadratic forms.

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The *three-dimensional* fragile lattice packings of spheres were determined by Fields (1980). There are only the simple cubic, simple hexagonal, body-centered cubic and body-centered tetragonal packings. Of these lattices, only the latter two are indecomposable: the simple cubic is the orthogonal sum of three one-dimensional lattices, and the simple hexagonal lattice is