or, as for example in protein structure work, of *the resolution* $\lambda/(2\sin\theta)_{\max}$, whenever experimental electron density maps are published.

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X-ray Diffraction from a $6H$ Structure Containing Intrinsic Faults

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The theory of X-ray diffraction from a one-dimensionally disordered $6H$ structure ($ABCACB$) containing a random distribution of 14 unique intrinsic fault configurations has been developed. An exact expression for the diffracted intensity has been derived in terms of the coefficients of the characteristic equation and the boundary conditions by applying Holloway's method of analytic solution. This expression is then used to obtain the diffracted intensity in reciprocal space as a function of the 14 fault probabilities, assuming these to be small. Observable diffraction effects like peak broadening, peak shift and the change in the peak intensity are discussed for different single-crystal reflexions. A unique evaluation of all 14 fault probabilities is not possible from an experimental measurement of diffraction effects. However, it is often possible to neglect certain fault probabilities on the basis of physical considerations such as the stacking-fault energy and the mechanism of formation of faults in the $6H$ structure.

Introduction

Recently we have shown (Pandey & Krishna, 1975*a*, *b*, *c*, *d*) that all the observed polytype structures in lead iodide, cadmium iodide and silicon carbide can result from spiral growth round a single screw dislocation created in a basic structure containing random stacking faults. The basic structures, which are the more commonly found small-period modifications, are different in different materials (Verma & Krishna, 1966). Thus the basic structure in PbI_2 is type $2H(A\gamma B)$; those in CdI_2 are $2H(A\gamma B)$ and $4H(A\gamma BC\alpha B)$ while those in SiC are $6H(A\alpha B\beta C\gamma A\alpha C\gamma B\beta)$, $15R(A\alpha B\beta C\gamma B\beta A\alpha B\beta C\gamma A\alpha C\gamma B\beta C\gamma A\alpha B\beta A\alpha C\gamma)$ and $4H(A\alpha B\beta C\gamma B\beta)$. The range of interaction, as defined by Jagodzinski (1949*a*), extends to two, three, four and six layers for the $2H$, $4H$, $6H$ and $15R$ structures respectively. Stacking-fault energy in all these materials is very low (Stevens, 1972; Prasad & Srivastava, 1970) and the basic structures frequently contain a random distribution of stacking faults. This produces diffuse streaks connecting X-ray diffraction maxima that originate from reciprocal-lattice rows parallel to $\mathbf{c}^*$. The concentration of stacking faults varies considerably from one crystal to another but the average value of the fault-order degree, as measured experimentally, is reported to be 0·12 for SiC and 0·26 for CdI_2 (Jagodzinski, 1954; Jain & Trigunayat, 1970). The theory of X-ray diffraction from randomly faulted close-packed structures with a range of interaction up to three layers has been developed by several workers (Wilson, 1942; Hendricks & Teller, 1942; Jagodzinski, 1949*a*, *b*; Paterson, 1952; Gevers, 1954; Kakinoki & Komura, 1952; Kakinoki, 1967; Johnson, 1963; Holloway, 1969; Prasad & Lele, 1971).

Gevers (1954) has developed the theory of X-ray diffraction from close-packed structures with a four-layer range of interaction. Lele (1974*a*, *b*, *c*) has extended the theory to a stage where the fault probabilities are directly related to the experimentally observable diffraction effects for the structures $6H$, $9R$ and $12R$. We have shown in an earlier publication that there are 18 possible intrinsic fault configurations that can occur in the $6H$ structure (Pandey & Krishna, 1975*c*, *d*). Of these G_5^{6H}, G_7^{6H}, G_{10}^{6H} and G_{15}^{6H} are enantiomorphous with G_{14}^{6H}, G_9^{6H}, G_{13}^{6H} and G_{18}^{6H} leaving only 14 unique intrinsic fault configurations (for notations see Pandey & Krishna, 1975*c*, *d*). Gevers (1954) and Lele (1974) have considered only the fault configurations G_1^{6H}, G_3^{6H}, G_4^{6H}, G_7^{6H} and G_{16}^{6H} to occur in the 6*H* structure. This assumption is not justified since the other fault configurations can also occur depending on the manner in which the disordered 6*H* structure is obtained. For example, the fault configurations that are likely to occur in a _6*H* SiC crystal obtained directly from a growth run would be very different from those that occur in a disordered 6*H* structure obtained by heating the silicon carbide 2*H* or 3*C* modifications until they undergo solid-state transformation to the 6*H* phase (Krishna & Marshall, 1971*a*, *b*).

In the present investigation we therefore consider X-ray diffraction from a 6*H* crystal containing all the 14 fault configurations and predict the effects that would be observable on single-crystal X-ray diffraction photographs. To do this the characteristic equation has been obtained by the method developed by Prasad & Lele (1971) but the final intensity expression is deduced by Holloway's (1969) method of analytic solution which expresses the diffracted intensity in terms of the coefficients of the characteristic equation and the boundary conditions. This obviates the necessity of explicitly solving the characteristic equation and considerably simplifies the calculations. Moreover one obtains an exact expression for the diffracted intensity which can be used to compute numerically observable diffraction effects even in the case of strongly disordered crystals (with large α values). Diffraction effects expected from disordered single crystals with small values of α have been predicted and the equations can be used for experimental determination of the concentration of different types of faults present in disordered 6*H* structures obtained by different methods.

General expression for the diffracted intensity

Following the notations used by Warren (1959), the diffracted intensity from a faulted close-packed 6*H* structure can be written as

$$I(h_3)=\sum_{m=-\infty}^{\infty}\psi^2\langle\exp[i\varphi_m]\rangle\exp\left[\frac{m2\pi ih_3}{6}\right],\qquad(1)$$

where φ_m is the phase difference across a pair of *m*th neighbour layers and is given by

$$\varphi_m=\frac{2\pi}{3}(H_0-K_0)q_m\,,\qquad(2)$$

q_m being the displacement of the *m*th layer with respect to the original layer in units of $\frac{1}{6}\langle10\bar{1}0\rangle$ in a plane parallel to the layers. It is known (Prasad & Lele, 1971) that

$$\langle\exp[i\varphi_m]\rangle=\sum_{j=1}^{n}C_j\varrho_j^m\,,$$

where ϱ_j are the roots of the so-called characteristic equation, which in general has the form

$$a_n\varrho^n+a_{n-1}\varrho^{n-1}+\ldots+a_0=0\,.\qquad(3)$$

From equations (3) and (1), we obtain the diffracted intensity as

$$I(h_3)=\sum_{j=1}^{n}\left[C_j+\frac{C_j\varrho_j}{\exp\left[\frac{-i\pi h_3}{3}\right]-\varrho_j}+\frac{C_j\varrho_j}{\exp\left[\frac{i\pi h_3}{3}\right]-\varrho_j}\right].\qquad(4)$$

In summing the geometric series we have assumed that none of the roots of equation (3) have unit modulus. Following Holloway (1969), equation (4) can now be written as:

$$I(h_3)=\left[\frac{1}{2}+\frac{\sum_{j=1}^{n-1}\sum_{k=0}^{j-1}a_{n-k}J(j-k)\exp\left[(n-j)\frac{i\pi h_3}{3}\right]-a_0}{\sum_{j=0}^{n}a_j\exp\left[\frac{ji\pi h_3}{3}\right]}\right]+(\text{complex conjugate})\,,\qquad(5)$$

where

$$\sum_{j=1}^{n}C_j=\langle\exp[i\varphi_0]\rangle=J(0)=1\,;$$

and

$$a_n=1\,.$$

For a 6*H* crystal with intrinsic faults, the characteristic equation is of sixth degree so that the diffracted intensity can be written as:

$$I(h_3)=1+\frac{2\sum_{m=0}^{6}N_m\cos\left[\frac{m\pi h_3}{3}\right]}{\sum_{m=0}^{6}D_m\cos\left[\frac{m\pi h_3}{3}\right]}\,,\qquad(6)$$

where

$$D_0=(1+a_5^2+a_4^2+a_3^2+a_2^2+a_1^2+a_0^2)\,;$$
$$D_1=2(a_5+a_5a_4+a_4a_3+a_3a_2+a_2a_1+a_1a_0)\,;$$
$$D_2=2(a_4+a_5a_3+a_4a_2+a_3a_1+a_2a_0)\,;$$
$$D_3=2(a_3+a_5a_2+a_4a_1+a_3a_0)\,;$$
$$D_4=2(a_2+a_5a_1+a_4a_0)\,;$$
$$D_5=2(a_1+a_5a_0)\,;$$
$$D_6=2a_0\,,$$

and

$$\begin{aligned}N_0={}&a_5J(1)+a_4[J(2)+a_5J(1)]+a_3[J(3)+a_5J(2)\\&+a_4J(1)]+a_2[J(4)+a_5J(3)+a_4J(2)+a_3J(1)]\\&+a_1[J(5)+a_5J(4)+a_4J(3)+a_3J(2)+a_2J(1)]-a_0^2\,.\end{aligned}$$

$$\begin{aligned}N_1={}&(1+a_4)J(1)+(a_5+a_3)\,[J(2)+a_5J(1)]\\&+(a_4+a_2)\,[J(3)+a_5J(2)+a_4J(1)]\\&+(a_3+a_1)\,[J(4)+a_5J(3)+a_4J(2)+a_3J(1)]\\&+(a_2+a_0)\,[J(5)+a_5J(4)+a_4J(3)+a_3J(2)+a_2J(1)]\\&-a_1a_0\,.\end{aligned}$$

$$\begin{aligned} N_2 = {} & a_3J(1)+(1+a_2)\,[J(2)+a_5J(1)] \\ & +(a_5+a_1)\,[J(3)+a_5J(2)+a_4J(1)] \\ & +(a_4+a_0)\,[J(4)+a_5J(3)+a_4J(2)+a_3J(1)] \\ & +a_3[J(5)+a_5J(4)+a_4J(3)+a_3J(2)+a_2J(1)] \\ & -a_2a_0\,. \end{aligned}$$

$$\begin{aligned} N_3 = {} & a_2J_1+a_1[J(2)+a_5J(1)] \\ & +(1+a_0)\,[J(3)+a_5J(2)+a_4J(1)] \\ & +a_5[J(4)+a_5J(3)+a_4J(2)+a_3J(1)] \\ & +a_4[J(5)+a_5J(4)+a_4J(3)+a_3J(2)+a_2J(1)] \\ & -a_3a_0\,. \end{aligned}$$

$$\begin{aligned} N_4 = {} & a_5[J(5)+a_5J(4)+a_4J(3)+a_3J(2)+a_2J(1)] \\ & +a_1J(1)+a_0[J(2)+a_5J(1)] \\ & +[J(4)+a_5J(3)+a_4J(2)+a_3J(1)]-a_4a_0\,. \end{aligned}$$

$$N_5=a_0J_1+[J(5)+a_5J(4)+a_4J(3)+a_3J(2)+a_2J(1)]\,.$$

$$N_6=-a_0\,.$$

Thus we need to evaluate the coefficients a_j of the characteristic equation and the boundary conditions $J(j)$ to obtain the final expression for the diffracted intensity.

Characteristic equation for faulted 6*H*

To get the characteristic equation we shall follow the method developed by Prasad & Lele (1971). Six kinds of layers need to be distinguished in the perfect 6*H* (*hkkhkk*) structure of which three layers have a stacking offset $+S$ with respect to the preceding layer and the remaining three an offset $-S$. Let us choose the origin on an *h*-type layer which is followed by two *k* layers such that the layer next to the origin has a stacking offset $+S$. Let the layer through the origin be denoted by a subscript 0 and succeeding layers in the unit cell by subscripts 1, 2, 3, 4 and 5. Then the perfect 6*H* structure can be written as

$$\begin{array}{cccccccccccc} h & k & k & h & k & k & h & k & k & h & k & k \\ A_0 & B_1 & C_2 & A_3 & C_4 & B_5 & A_0 & B_1 & C_2 & A_3 & C_4 & B_5 \\ & +S & +S & +S & -S & -S & -S & +S & +S & +S & -S & -S \;. \end{array}$$

The function $J(m,j)=\langle\exp\,[i\varphi_m]_j\rangle$, as defined by Prasad & Lele (1971), may be written as

$$J(m,j)=\sum_j P(m,j)\exp\,[i\varphi_m]_j\,,$$

where $P(m,j)$ is the probability of finding an mth layer with the subscript j mod 6 and $[\varphi_m]_j$ is the phase difference of the mth layer with subscript j mod 6. $J(m,j)$ can now be related to α_i, the probability of occurrence of a fault of type G_i^{6H}, with the help of Fig. 1 which considers the transition probabilities for going from the $(m-1)$th layer to the mth layer. The subscripts can be found from the relative positions of different layers. The set of six coupled difference equations for $J(m,j)$ so obtained may be solved by writing $J(m,j)=C_j\varrho^m$, where C_j and ϱ are the functions of α. After eliminating the constants C_j, we finally obtain the following characteristic equation:

$$\begin{aligned} & \varrho^6+(\alpha_3+2\alpha_{15})\varrho^5 \\ & +(\alpha_2-2\alpha_6-2\alpha_{17}+\alpha_3^2-\alpha_4^2-\alpha_8^2-\alpha_{11}^2+3\alpha_{15}^2)\varrho^4 \\ & +[2\alpha_5(1-\alpha_5)-2\alpha_{12}+2\alpha_{15}^3]\varrho^3 \\ & +[-\alpha_1^2+\alpha_2^2+\alpha_4(1-\alpha_4)+\alpha_6^2-2\alpha_8(1-\alpha_8) \\ & -\alpha_{10}^2(2-\alpha_{10})^2+\alpha_{11}(1-\alpha_{11})+\alpha_{17}^2+\alpha_{15}^4]\varrho^2 \\ & +[\alpha_1(1-\alpha_1)-2\alpha_{10}(2-\alpha_{10})\,(1-\alpha_{10})^2]\varrho \\ & -[(1-\alpha_1)^2+(1-\alpha_2)^2+(1-\alpha_3)^2+(1-\alpha_4)^2 \\ & -2\alpha_5^2(1-\alpha_5)^2+(1-\alpha_6)^2+3\alpha_7^2(1-\alpha_7)^2+(1-\alpha_8)^2 \\ & +(1-\alpha_{11})^2+(1-\alpha_{12})^2+(1-\alpha_{16})^2+(1-\alpha_{17})^2 \\ & -\alpha_{12}^2-\alpha_{16}(1-\alpha_{16})+\alpha_5^3-(1-\alpha_5)^4-2\alpha_7^3(1-\alpha_7) \\ & -2\alpha_7(1-\alpha_7)^3+\alpha_7^4+(1-\alpha_7)^4+(1-\alpha_{10})^4 \\ & +(1-\alpha_{15})^4-13]=0\,. \end{aligned} \tag{7}$$

Evaluation of boundary conditions

Boundary conditions will be evaluated in two steps by the method given by Prasad & Lele (1971). First one obtains the probability, w_j, of finding a layer with a particular value of j on passing through an arbitrary region of the crystal. Then considering all possible sequences starting with A_0, B_1, C_2, A_3, C_4 and B_5, one obtains

$$J(m)=\langle\exp\,[i\varphi_m]\rangle=\sum_{j=0}^{5} w_j\langle\exp\,[i\varphi_m^{x_j}]\rangle\,, \tag{8}$$

where x_j denotes the layer type at the origin. From Fig. 1, one can obtain the following values for the w's:

$$\begin{aligned} w_0=w_3=\tfrac{1}{6}[1-\tfrac{1}{3}(& 2\alpha_1-\alpha_2-2\alpha_3+\alpha_4-\alpha_6+\alpha_8-2\alpha_{10} \\ & -2\alpha_{11}+2\alpha_{15}+2\alpha_{17})] \end{aligned} \tag{9}$$

$$\begin{aligned} w_1=w_4=\tfrac{1}{6}[1+\tfrac{1}{3}(& \alpha_1-2\alpha_2-\alpha_3+2\alpha_4+\alpha_6-\alpha_8-\alpha_{10} \\ & -\alpha_{11}+\alpha_{15}+\alpha_{17})] \end{aligned} \tag{10}$$

$$\begin{aligned} w_2=w_5=\tfrac{1}{6}[1+\tfrac{1}{3}(& \alpha_1+\alpha_2-\alpha_3-\alpha_4-2\alpha_6+2\alpha_8-\alpha_{10} \\ & -\alpha_{11}+\alpha_{15}+\alpha_{17})]\,. \end{aligned} \tag{11}$$

These values were used for evaluating the boundary conditions, $J(0)$, $J(1)$, $J(2)$, $J(3)$, $J(4)$ and $J(5)$ given below:

$$J(0)=1 \tag{12}$$

$$J(1)=-\tfrac{1}{2} \tag{13}$$

$$\begin{aligned} J(2)=\tfrac{1}{6}[& \alpha_1-2\alpha_2-\alpha_3+2\alpha_4+6\alpha_5+4\alpha_6+2\alpha_8+\tfrac{8}{3}\alpha_{10} \\ & -4\alpha_{11}-3\alpha_{12}+10\alpha_{15}+6\alpha_{16}+4\alpha_{17}] \end{aligned} \tag{14}$$

$$\begin{aligned} J(3)=\tfrac{1}{6}[& -2\alpha_1+4\alpha_2+2\alpha_3-\alpha_4-6\alpha_5-2\alpha_6-4\alpha_8+2\alpha_{10} \\ & +8\alpha_{11}+6\alpha_{12}-8\alpha_{15}-3\alpha_{16}-5\alpha_{17}] \end{aligned} \tag{15}$$

$$J(4)=\tfrac{1}{6}[4\alpha_1-2\alpha_2-\alpha_3-4\alpha_4-2\alpha_6+6\alpha_7+8\alpha_8-10\alpha_{10} -4\alpha_{11}-3\alpha_{12}+4\alpha_{15}+4\alpha_{17}] \tag{16}$$

$$J(5)=\tfrac{1}{6}[-3+6\alpha_2+6\alpha_3+9\alpha_4+12\alpha_5+6\alpha_6+12\alpha_7 +30\alpha_{10}+6\alpha_{11}+6\alpha_{12}+6\alpha_{15}+6\alpha_{16}+3\alpha_{17}]\,. \tag{17}$$

Substituting the values of a_j from equation (7) and $J(j)$ from equations (12) to (17) in equation (6), one finally obtains the expression for diffracted intensity.

Deduction of diffraction effects

The intensity maxima occur near the positions for which $L(=h_3)=1$, 2, 3, 4 and 5. Setting $\pi h_3/3=(\pi/3\pm\pi\Delta h_3/3)$, $(2\pi/3\pm\pi\Delta h_3/3)$ and $(\pi\pm\pi\Delta h_3/3)$ corresponding to the peak positions of reflexions with $L=6M\pm1$, $6M\pm2$ and $6M\pm3$ respectively in the intensity expression given by equation (7) and assuming α_i and $\Delta h_3\ll1$, one can find the expressions for the maximum intensity, $I_{\max}$, and the peak shift, Δh_3, by differentiating the equation (7) with respect to h_3 and equating to zero. With the values of $I_{\max}$, the half width, $|w|$, of the diffraction profile can be easily calculated. The results are given below:

$$I_{\max}\simeq2\psi^2/(5\alpha_1+3\alpha_2+5\alpha_3+3\alpha_4+4\alpha_5+6\alpha_6+12\alpha_7+6\alpha_8 +4\alpha_{10}+3\alpha_{11}+8\alpha_{12}+10\alpha_{15}+6\alpha_{16}+6\alpha_{17}) \tag{18}$$

for $L=6M\pm1$

$$I_{\max}\simeq2\psi^2/(\alpha_1+\alpha_2+\alpha_3+\alpha_4+4\alpha_5+2\alpha_6+4\alpha_7+2\alpha_8 +4\alpha_{10}+\alpha_{11}+2\alpha_{15}+2\alpha_{16}+2\alpha_{17}) \tag{19}$$

for $L=6M\pm2$, and

$$I_{\max}\simeq4\psi^2/(\alpha_1+3\alpha_2+\alpha_3+3\alpha_4+2\alpha_5+6\alpha_7+8\alpha_{10}+3\alpha_{11} +4\alpha_{12}+2\alpha_{15}+3\alpha_{16}) \tag{20}$$

for $L=6M\pm3$.

$$\Delta h_3\simeq\pm(\sqrt{3}/4\pi)\,(-\alpha_1+\alpha_2+\alpha_3-\alpha_4-2\alpha_6+2\alpha_8+4\alpha_{10} -\alpha_{11}+2\alpha_{15}-2\alpha_{17})\,, \tag{21}$$

for $L=6M\mp1$,

$$\Delta h_3\simeq\pm(\sqrt{3}/4\pi)\,(-\alpha_1-\alpha_2+\alpha_3+\alpha_4+2\alpha_6-2\alpha_8+4\alpha_{10} +\alpha_{11}+2\alpha_{15}+2\alpha_{17})\,, \tag{22}$$

for $L=6M\mp2$

and

$$\Delta h_3=0$$

for $L=6M\pm3$;

$$W_1\simeq\tfrac{1}{6}(5\alpha_1+3\alpha_2+5\alpha_3+3\alpha_4+4\alpha_5+6\alpha_6+12\alpha_7+6\alpha_8 +4\alpha_{10}+3\alpha_{11}+8\alpha_{12}+10\alpha_{15}+6\alpha_{16}+6\alpha_{17})\,, \tag{23}$$

for $L=6M\pm1$,

$$W_2\simeq\tfrac{1}{2}(\alpha_1+\alpha_2+\alpha_3+\alpha_4+4\alpha_5+2\alpha_6+4\alpha_7+2\alpha_8+4\alpha_{10} +\alpha_{11}+2\alpha_{15}+2\alpha_{16}+2\alpha_{17})\,, \tag{24}$$

for $L=6M\pm2$,

and

$$W_3\simeq\tfrac{1}{3}(\alpha_1+3\alpha_2+\alpha_3+3\alpha_4+2\alpha_5+6\alpha_7+8\alpha_{10}+3\alpha_{11} +4\alpha_{12}+2\alpha_{15}+3\alpha_{16})\,, \tag{25}$$

for $L=6M\pm3$.

The diffraction effects from a faulted $6H$ structure can be summarized as follows:

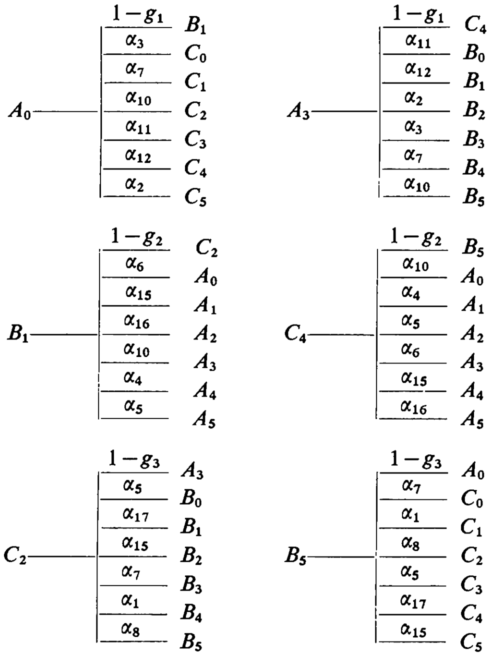
(i) Reflexions with $H-K=3N$ are unaffected by faulting.

(ii) All reflexions with $H-K\neq3N$ are broadened as a result of faulting.

(iii) There is change in the intensity of the peak maxima.

(iv) Reflexions with $H-K\neq3N$, $L=6M\pm1$ and $L=6M\pm2$ exhibit peak shifts also.

These results are in agreement with those obtained by Lele (1974*a*) for the fault configurations G_1^{6H}, G_3^{6H}, G_4^{6H}, G_7^{6H} and G_{16}^{6H}.



$$g_1=(\alpha_2+\alpha_3+\alpha_7+\alpha_{10}+\alpha_{11}+\alpha_{12})$$
$$g_2=(\alpha_4+\alpha_5+\alpha_6+\alpha_{10}+\alpha_{15}+\alpha_{16})$$
$$g_3=(\alpha_1+\alpha_5+\alpha_7+\alpha_8+\alpha_{15}+\alpha_{16})$$

Fig. 1. Probability trees for successive layers.

Discussion and results

There are 14 unique intrinsic fault configurations in the $6H$ structure and only seven experimentally observable compound fault parameters [see equations (18) to (25)]. One can find expressions for two more experimentally observable parameters from peak asymmetry measurements. The changes in the integrated intensity can be used as a measure of faulting instead of changes in the peak maxima. But the peak asymmetry and changes in integrated intensities are usually too small to be estimated experimentally with sufficient accuracy. Thus peak shift and half width appear to be the best measures of faulting. These provide us with only five compound fault parameters from which a unique evaluation of all the 14 unknowns is not possible.

However, it is usually possible to neglect some of the α's which are expected to have very low values on the basis of physical considerations. For example, it is well known that in the α-SiC crystals grown at high temperatures, fault configurations containing $h-h$ contacts are unstable and do not occur (Krishna & Marshall, 1971*a*, *b*). Consequently we can take $\alpha_4=\alpha_5=\alpha_6=\alpha_{10}=\alpha_{15}=\alpha_{16}=\alpha_{17}=0$. In the case of such as-grown crystals the relative magnitudes of the remaining seven α's will depend on the relative stacking-fault energies (SFE) of the corresponding fault configurations. These were evaluated by us in earlier papers (Pandey & Krishna, 1975*c*, *d*) where it was shown that the SFE of the fault configurations G_1^{6H}, G_2^{6H}, G_3^{6H}, G_7^{6H} and G_8^{6H} is much less than that of G_{11}^{6H} and G_{12}^{6H}. It is therefore to be expected that α_1, α_2, α_3, α_7 and α_8 will have much larger values than α_{11} and α_{12} in as-grown 6*H* SiC crystals. If the latter are neglected, we are left with only five unknowns whose value can be experimentally determined by using equations (18) to (25).

The above arguments are not applicable to a disordered 6*H* structure obtained from a 2*H* SiC crystal by solid-state transformation. Krishna & Marshall (1971*a*, *b*) have shown that the transformation occurs by a disordering process and the end product is invariably a faulted 6*H* structure. Such a structure would also contain fault configurations involving $h-h$ contacts between the layers. The fault probabilities α_4, α_5, α_6, α_{10}, α_{15}, α_{16} and α_{17} must then be taken into account.

It should be noted that equation (5) is subject to the usual assumptions about crystal size and the extent and spacing of the faulted close-packed planes, but otherwise its generality is restricted only by the condition that none of the roots of the characteristic equation has unit modulus (Holloway, 1969). Thus, in the special case when only one of the fault configurations G_{12}^{6H}, G_6^{6H} or G_{17}^{6H} is present, the above deduction will not be valid since $\varrho=\pm1$ becomes a root of the characteristic equation. It was pointed by Jagodzinski (1954) that roots with unit modulus represent a long-range correlation between the positions of close-packed layers and add a sharply peaked component to certain X-ray reflexions. However, in the case of α-SiC, this will be a rare eventuality since the fault configurations G_6^{6H} and G_{17}^{6H} contain $h-h$ contact and the fault configuration G_{12}^{6H} has a high SFE $3\psi_2$ (for notations see Pandey & Krishna, 1975*c*, *d*). None of the three fault configurations is therefore likely to occur by itself in α-6*H* SiC crystals. The characteristic equation and the expression for observable diffraction effects have been obtained for small values of α *i.e.* $\alpha_i \ll 1$. This assumption is not valid in the case of heavily faulted 6*H* SiC structures such as those obtained from the 2*H* or 3*C* crystals by solid-state transformations. In such cases it is necessary to perform a more rigorous calculation including higher-order terms in α using the exact intensity expression given by equation (6), which is valid for all values of α.

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