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X-ray Diffraction from Double Hexagonal Close-Packed Crystals with Stacking Faults

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The general theory of X-ray diffraction by double hexagonal close-packed crystals with stacking faults is developed. The intensity distribution in reciprocal space is derived as a function of nine parameters which represent the fault probabilities. Only reflexions with $H-K\neq 0$ mod 3 are affected. For these, there are generally changes in peak integrated intensity and peak broadening. In addition, reflexions with $L=\pm 1$ mod 4 exhibit peak shift and peak asymmetry. It is shown that seven independent combinations of the fault parameters can be evaluated from the measured profile characteristics.

Introduction

This work forms a part of a programme of study of imperfections, particularly stacking faults, in double hexagonal close-packed (d.h.c.p.) crystals. This structure can be considered as a layer structure produced by the regular stacking of its basal planes. Possible deviations in the regular ... *ABAC* ... stacking sequence have been considered by Lele, Prasad & Rama Rao (1969; 1970). Seven intrinsic and two extrinsic faults are of interest. The fault vector, **R**, which represents the displacement due to the fault is given in Table 1, for all nine faults. We note that intrinsic *c*, 2*c*, 3*c* and extrinsic 4*c* faults can occur only after *h* type layers while intrinsic *h*, 2*h*, 3*h* faults can occur only after *c* type layers. Intrinsic *ch* and extrinsic *cch* faults can, however, occur after either type of layer. *c* and *h* respectively denote the cubic and hexagonal configuration of a layer. The structures resulting due to the introduction of faults of one type successively are also indicated in Table 1. Further, the numbers of layers common to the regions on either side of a fault are respectively 2, 1 and 0 for intrinsic *c* and *h* faults, intrinsic 2*c* and 2*h* faults, and intrinsic 3*c*, 3*h* and *ch* faults. For extrinsic 4*c* and *cch* faults, one layer called an extra-ordinary layer does not belong to either region on the two sides of a fault.

Diffraction by intrinsic *c* and *h* faults, which are 'growth' faults with a three layer range of interaction, was first considered by Jagodzinski (1949) and subsequently by Kakinoki & Komura (1952), Allegra (1964) and Kakinoki (1967). These treatments have, however, not been carried far enough to relate the diffraction theory to experimentally observable characteristics of a d.h.c.p. powder pattern. Diffraction by intrinsic *ch* faults, which are 'deformation' faults, has been considered by Gevers (1954) and by Lele, Prasad & Anantharaman (1969). Intrinsic 3*c* faults in d.h.c.p. crystals can be alternatively regarded as extrinsic 3*c* faults in h.c.p. crystals. Diffraction effects due to these faults have been found by Lele, Anantharaman & Johnson (1967) and by Holloway (1969). In the present paper, we shall consider X-ray diffraction from d.h.c.p. crystals with the nine types of stacking faults mentioned above. The earlier treatments of Jagodzinski (1949), Gevers (1954) and Lele *et al.* (1967) form special cases. The mathematical procedure utilized for the solution is an extension of that of Lele (1969) in which difference equations, relating adjacent layers only, are first formulated. This approach avoids an over-specification of the problem and thus possible errors. We shall first find the intensity distribution in reciprocal space and then give expressions for measurable characteristics of the fault profiles. The calculations are subject to the following assumptions:

1. The fault probabilities are small (usually these values are of physical interest and the assumption obviates consideration of the simultaneous occurrence of faults).
2. The crystal is infinite in size and free of distortion.
3. The scattering power is the same for all the close-packed layers in case of alloys.
4. There is no change in the lattice spacing at the faults.
5. The faults are distributed at random.
6. The faults extend over entire domains.

General expression for diffracted intensity

In terms of hexagonal basis vectors $\mathbf{A}_1$, $\mathbf{A}_2$, $\mathbf{A}_3$, the position vector of (m_1, m_2) atom in the m_3 layer of a possibly faulted d.h.c.p. crystal is

$$R_m=m_1\mathbf{A}_1+m_2\mathbf{A}_2+\tfrac{1}{4}\,.\,m_3\mathbf{A}_3+\mathbf{S}\,.\,q_{m_3} \tag{1}$$

where the stacking off-set vector

$$\mathbf{S}=\tfrac{1}{3}\,(\mathbf{A}_1-\mathbf{A}_2) \tag{2}$$

and is identical with the glide vector **S** in Table 1. Expressing vectors in reciprocal space in terms of the vectors $\mathbf{B}_1$, $\mathbf{B}_2$, $\mathbf{B}_3$ reciprocal to $\mathbf{A}_1$, $\mathbf{A}_2$, $\mathbf{A}_3$ and continuous variables h_1, h_2, h_3, the diffracted intensity is given by (Warren, 1959)

$$I(h_3)=\psi^2\sum_{m=-\infty}^{\infty}\langle\exp[2\pi i(H\mathbf{B}_1+K\mathbf{B}_2+h_3\mathbf{B}_3)\,.\,\mathbf{S}(q_{m_3}-q_{m_3'})]\rangle\exp[2\pi i\,mh_3/4]$$

$$= \psi^2 \sum_{m=-\infty}^{\infty} \langle \exp [i\Phi_m] \rangle \exp [\pi i m h_3/2] \quad (3)$$

where ψ^2 is a function of h_1 and h_2 which vanishes except when $h_1 = H$ and $h_2 = K$. The phase difference Φ_m is given by

$$\Phi_m = \frac{2\pi}{3} (H-K)(q_{m_3} - q_{m'_3}) = \varphi_0(H-K) q_m \quad (4)$$

where $\varphi_0 = (2\pi/3)$. From equations (3) and (4), it is clear that only reflexions with $H-K \neq 0$ mod 3 are affected by faulting. We shall concern our selves further only with reflexions with $H-K=1$ mod 3 since the case $H-K=2$ mod 3 is equivalent to it.

Diffraction from faulted crystals

The essential problem in finding the intensity distribution in reciprocal space is the evaluation of $\langle \exp [i\Phi_m] \rangle$ [see equation (3)]. There are several equivalent approaches to a solution of this problem (Wilson, 1942; Hendricks & Teller, 1942; Méring, 1949; Johnson, 1963). Our approach is outlined in the following. Let $P(\Phi_m)$ be the probability of obtaining a phase difference Φ_m between the mth layer and the origin layer in an m-layer sequence in the faulted crystal, then

$$\langle \exp [i\Phi_m] \rangle = \sum P(\Phi_m) \exp [i\Phi_m] . \quad (5)$$

Therefore we shall find (1) an expression for Φ_m in terms of the numbers of faults of different types in the sequences and (2) a recurrence relation for $P(\Phi_m)$ in terms of the fault probabilities. On substitution of these two relations in equation (5), we obtain a recurrence relation for $\langle \exp [i\Phi_m] \rangle$. Utilizing initial conditions, *i.e.* values of $\langle \exp [i\Phi_m] \rangle$ for $m=0$ to 4 obtained by a consideration of all possible sequences up to $m=4$, we get a solution for the recurrence relation in $\langle \exp [i\Phi_m] \rangle$. Substitution of this solution in the intensity equation (3) yields the intensity distribution in reciprocal space explicitly in terms of the fault probabilities.

In the perfect d.h.c.p. structure, we distinguish four types of layers characterized in that (1) they are in a c or h configuration, (2) the stacking off-set to the succeeding layer is $+\mathbf{S}$ or $-\mathbf{S}$. We choose any c type layer as the origin layer such that the stacking off-set from this layer to the next is $+\mathbf{S}$. To distinguish it we give a subscript 0, as in A_0. The other layers are now numbered consecutively and the layer n has a subscript $j=n$ mod 4. Thus the perfect d.h.c.p. structure may be represented as

$$\begin{array}{cccccccccccccccc}
c & & h & & c & & h & & c & & h & & c & & h \\
A_0 & & B_1 & & A_2 & & C_3 & & A_0 & & B_1 & & A_2 & & C_3 \\
& +\mathbf{S} & & -\mathbf{S} & & -\mathbf{S} & & +\mathbf{S} & & +\mathbf{S} & & -\mathbf{S} & & -\mathbf{S} &
\end{array}$$

$$\begin{array}{cccccccccccccccc}
c & & h & & c & & h & & c & & h & & c & & h \\
B_0 & & C_1 & & B_2 & & A_3 & & B_0 & & C_1 & & B_2 & & A_3 \\
& +\mathbf{S} & & -\mathbf{S} & & -\mathbf{S} & & +\mathbf{S} & & +\mathbf{S} & & -\mathbf{S} & & -\mathbf{S} &
\end{array}$$

$$\begin{array}{cccccccccccccccc}
c & & h & & c & & h & & c & & h & & c & & h \\
C_0 & & A_1 & & C_2 & & B_3 & & C_0 & & A_1 & & C_2 & & B_3 \\
& +\mathbf{S} & & -\mathbf{S} & & -\mathbf{S} & & +\mathbf{S} & & +\mathbf{S} & & -\mathbf{S} & & -\mathbf{S} &
\end{array}$$

where we have indicated the configuration (c or h) of the layer, the stacking off-set vector ($+\mathbf{S}$ or $-\mathbf{S}$) and the appropriate subscript. We note that the subscript to a layer is uniquely related to the stacking off-set vector.

In faulted crystals, there are six types of layers besides the four considered above. As already noted, one layer called an extra-ordinary layer does not belong to either region on the two sides of an extrinsic $4c$ fault as also an extrinsic cch fault. This extra-ordinary layer is designated B_3^{e1} or C_1^{e1} respectively according as it occurs after a C_3 or B_1 layer for extrinsic $4c$ faults. For extrinsic cch faults, we designate the extra-ordinary layer C_0^{e2}, C_1^{e2}, B_2^{e2}, B_3^{e2} according as it occurs after an A_0, B_1, A_2, C_3 layer respectively.

We shall first consider sequences which begin and end with ordinary layers. In a perfect crystal, let the phase difference in an n-layer sequence starting with a layer of type X be Φ_n^X. For a sequence starting with A_0 type layer, we have

$$\Phi_n^{A_0} = \tfrac{1}{2} [1-(-1)^n] \times i^{n-1} . \varphi_0 , \quad n \geq 0 . \quad (6)$$

since the displacement $\pm\mathbf{S}$ corresponds to the phase shift $\pm\varphi_0$ and $i=\sqrt{-1}$. We now, consider the effect of introducing k^c intrinsic c, k^h intrinsic h, k^{2c} intrinsic $2c$, k^{2h} intrinsic $2h$, k^{3c} intrinsic $3c$, k^{3h} intrinsic $3h$, k^{ch} intrinsic ch, k^{4c} extrinsic $4c$ and k^{cch} extrinsic cch faults.

Table 1. *Process of fault formation, fault vector and resultant structure on insertion of successive faults.*

Fault	Process of formation	Fault vector* $\mathbf{R}$	Resultant structure
Intrinsic-c	Insertion of 1 layer + Glide	$+\mathbf{F}\pm\mathbf{S}$	c
Intrinsic-h	Removal of 1 layer + Glide	$-\mathbf{F}\pm\mathbf{S}$	h
Intrinsic-$2c$	Insertion of 2 layers + Glide	$+2\mathbf{F}\pm\mathbf{S}$	c
Intrinsic-$2h$	Removal of 2 layers	$-2\mathbf{F}$	h
Intrinsic-$3c$	Removal of 1 layer	$-\mathbf{F}$	h
Intrinsic-$3h$	Insertion of 1 layer + Glide	$+\mathbf{F}\mp\mathbf{S}$	c
Intrinsic-ch	Glide	$\pm\mathbf{S}$	ch
Extrinsic-$4c$	Double glide	$\mp\mathbf{S}$	ch
Extrinsic-cch	Insertion of 1 layer	$+\mathbf{F}$	cch

* $\mathbf{F} = \frac{1}{4}[0001]$, $\mathbf{S} = \frac{1}{3}[1\bar{1}00]$.

Recalling the process of formation of these faults (Table 1), the first step in their formation consists in insertion of

$$K_i = k^c + 2k^{2c} + k^{3h} + k^{cch} \quad (7)$$

layers and removal of

$$K_r = k^h + 2k^{2h} + k^{3c} \quad (8)$$

layers. This changes the numbering of the layers so that the layer n in the perfect crystal becomes the layer m in the faulted crystal with

$$m = n + K_i - K_r . \quad (9)$$

The subscript of the layer m in the faulted crystal would thus be

$$j = n \bmod 4 = (m - K_i + K_r) \bmod 4 \quad (10)$$

The second step consists in gliding k^c, k^h, k^{2c}, k^{3h}, k^{ch}, k^{4c} layers through $\pm$S. The direction of glide depends on the value of j and is given in Table 2. Denoting the number of faults of type Y occurring at a particular value of j by k_j^Y, we have

$$k^Y = \sum_j k_j^Y \quad (11)$$

Table 2. *Dependence of glide vector on j value*

Fault	Value of j for glide through $+$S	$-$S
Intrinsic-c	3	1
Intrinsic-h	0	2
Intrinsic-2c	2	0
Intrinsic-3h	2	0
Intrinsic-ch	0, 1	2, 3
Extrinsic-4c	3	1

It follows that the glide operation gives rise to an additional phase shift of

$$\delta\Phi_{\text{glide}} = (K_p - K_n)\,\varphi_0 \quad (12)$$

where

$$K_p = k_1^c + k_0^h + k_2^{2c} + k_2^{3h} + k_0^{ch} + k_1^{ch} + k_3^{4c} \quad (13)$$

$$K_n = k_3^c + k_2^h + k_0^{2c} + k_0^{3h} + k_2^{ch} + k_3^{ch} + k_1^{4c} \quad (14)$$

From equations (6) to (14) and the above considerations, we obtain for the phase difference between the mth layer and the origin layer

$$\Phi_m^{A0} = [\tfrac{1}{2}\{1-(-1)^{m-K_i+K_r}\}\,(i)^{m-K_i+K_r-1} + (K_p - K_n)]\varphi_0,\ m \ge 0 . \quad (15)$$

Expressions for phase differences of sequences starting with B_1, A_2, C_3 type layers can be obtained similarly. Further, phase differences for m-layer sequences beginning and/or ending with extra-ordinary layers can be obtained from those for ordinary-ordinary $(m-1)$- or $(m-2)$-layer sequences respectively by adding extra-ordinary layers at either or both ends.

Let the probability of occurrence of a fault of type Y be α_Y and let the probability of obtaining an m-layer sequence having k^c, k^h, k^{2c}, k^{2h}, k^{3c}, k^{3h}, k^{ch}, k^{4c}, k^{cch} faults with origin at A_0 be $P(m, j, k^c, k^h, k^{2c}, k^{2h}, k^{3c}, k^{3h}, k^{ch}, k^{4c}, k^{cch})$, where j has been defined through equation (10). We shall abbreviate this to $P(m, j)$. Further, the probability of occurrence of a sequence with a change in any of the k's, *e.g.* $P(m, j, k^c-1, k^h, k^{2c}, k^{2h}, k^{3c}, k^{3h}, k^{ch}, k^{4c}, k^{cch})$ will be abbreviated to $P(m, j, k^c-1)$. To relate $P(m,j)$ and the α's, we consider the transition probabilities for going from the $(m-1)$th layer to the mth layer. As noted earlier, only intrinsic h, $2h$, $3h$, ch and extrinsic cch faults can occur after A_0 or A_2 layers with probabilities α_h, α_{2h}, α_{3h}, α_{ch} and α_{cch} respectively. The layer type following $A_0(A_2)$ layer in the absence of a fault is $B_1(C_3)$ occurring with probability $G_h(\alpha) = (1-\alpha_h-\alpha_{2h}-\alpha_{3h}-\alpha_{ch}-\alpha_{cch})$. Therefore, in the presence of a fault, the layer following $A_0(A_2)$ is $C(B)$. The subscript of the $C(B)$ layer can be found by considering the process of formation of the fault in addition to the usual change in $(m-1)$ to m in going from one layer to the next. For example, an intrinsic h fault occurring after an $A_0(A_2)$ layer involves removal of one layer with the subscript 1(3), hence the subscript of the layer following an $A_0(A_2)$ layer is 2(0) and thus the layer type is $C_2(B_0)$ as shown in Fig. 1(*a*) and (*c*). One can similarly obtain the subscript in the other cases. Again as noted earlier, only intrinsic c, $2c$, $3c$, ch and extrinsic $4c$, cch faults can occur after B_1 or C_3 layers with probabilities α_c, α_{2c}, α_{3c}, α_{ch}, α_{4c}, α_{cch} respectively. Thus the layer following $B_1(C_3)$, *viz.* $A_2(A_0)$, in the absence of a fault occurs with probability $G_c(\alpha) = (1-\alpha_c-\alpha_{2c}-\alpha_{3c}-\alpha_{ch}-\alpha_{4c}-\alpha_{cch})$. Consequently, the layer following $B_1(C_3)$ in the presence of a fault is $C(B)$. The subscripts can again be found from arguments similar to those advanced above. The transition probabilities from the four ordinary type layers and the six extra-ordinary type layers to the next possible layer are summarized in the probability trees in Fig. 1. From the Figure, we observe that an m-layer with the subscript $j=0$ can arise in the following six ways:

(1) From an $(m-1)$-layer with $j=0$ occurring with probability $P(m-1, 0, k_0^{3h}-1)$ followed by an intrinsic $3h$ fault occurring with probability α_{3h}.

(2) From an $(m-1)$-layer with $j=1$ occurring with probability $P(m-1, 1, k_0^{2c}-1)$ followed by an intrinsic $2c$ fault occurring with probability α_{2c}.

(3) From an $(m-1)$-layer with $j=2$ occurring with probability $P(m-1, 2, k_0^h-1)$ followed by an intrinsic h fault occurring with probability α_h.

(4) From an $(m-1)$-layer with $j=3$ occurring with probability $P(m-1, 3)$ followed by no fault with probability $G_c(\alpha)$.

(5) From an $(m-1)$-layer with $j=3$ occurring with probability $P(m-1, 3, k_0^{ch}-1)$ followed by an intrinsic ch fault occurring with probability α_{ch}.

(6) From an $(m-2)$-layer with $j=3$ occurring with probability $P(m-2, 3, k^{cch}-1)$ followed by an extrinsic cch fault occurring with probability α_{cch}.

The probability, $P(m, 0)$, of obtaining an m layer with $j=0$ is the sum of the probabilities of the above six events and is thus given by

$$\begin{aligned} P(m,0) = {} & (1-\alpha_c-\alpha_{2c}-\alpha_{3c}-\alpha_{ch}-\alpha_{4c}-\alpha_{cch})\,P(m-1,3) \\ & +\alpha_h P(m-1,2,k_0^h-1)+\alpha_{2c}P(m-1,1,k_0^{2c}-1) \\ & +\alpha_{3h}P(m-1,0,k_0^{3h}-1)+\alpha_{ch}P(m-1,3,k_0^{ch}-1) \\ & +\alpha_{cch}P(m-2,3,k^{cch}-1)\,, \qquad m\geq 2 \end{aligned} \tag{16}$$

Similarly,

$$\begin{aligned} P(m,1) = {} & (1-\alpha_h-\alpha_{2h}-\alpha_{3h}-\alpha_{ch}-\alpha_{cch})\,P(m-1,0) \\ & +\alpha_c P(m-1,1,k_1^c-1)+\alpha_{2h}P(m-1,2,k^{2h}-1) \\ & +\alpha_{3c}P(m-1,3,k^{3c}-1)+\alpha_{ch}P(m-1,0,k_1^{ch}-1) \\ & +\alpha_{4c}P(m-2,3,k_1^{4c}-1) \\ & +\alpha_{cch}P(m-2,0,k^{cch}-1)\,, \qquad m\geq 2 \end{aligned} \tag{17}$$

$$\begin{aligned} P(m,2) = {} & (1-\alpha_c-\alpha_{2c}-\alpha_{3c}-\alpha_{ch}-\alpha_{4c}-\alpha_{cch})\,P(m-1,1) \\ & +\alpha_h P(m-1,0,k_2^h-1)+\alpha_{2c}P(m-1,3,k_2^{2c}-1) \\ & +\alpha_{3h}P(m-1,2,k_2^{3h}-1)+\alpha_{ch}P(m-1,1,k_2^{ch}-1) \\ & +\alpha_{cch}P(m-2,1,k^{cch}-1)\,, \qquad m\geq 2 \end{aligned} \tag{18}$$

$$\begin{aligned} P(m,3) = {} & (1-\alpha_h-\alpha_{2h}-\alpha_{3h}-\alpha_{ch}-\alpha_{cch})\,P(m-1,2) \\ & +\alpha_c P(m-1,3,k_3^c-1)+\alpha_{2h}P(m-1,0,k^{2h}-1) \\ & +\alpha_{3c}P(m-1,1,k^{3c}-1)+\alpha_{ch}P(m-1,2,k_3^{ch}-1) \\ & +\alpha_{4c}P(m-2,1,k_3^{4c}-1) \\ & +\alpha_{cch}P(m-2,2,k^{cch}-1)\,, \qquad m\geq 2 \end{aligned} \tag{19}$$

Let us define

$$J(m,j)=\sum_{\text{All } k\text{'s}} P(m,j)\exp\,[i\Phi_m^{A_0}] \tag{20}$$

where the summation extends only over those values of the k's which correspond to a particular value of j. Consider the value of $J(m, 0)$. Substituting for $\Phi_m^{A_0}$ from equation (15) (with $j=0$) and for $P(m, 0)$ from equation (16) in equation (20), we have

$$\begin{aligned} J(m,0) = {} & \sum_{\text{All } k\text{'s}} \{(1-\alpha_c-\alpha_{2c}-\alpha_{3c}-\alpha_{ch}-\alpha_{4c}-\alpha_{cch}) \\ & \times P(m-1,3)+\alpha_h P(m-1,2,k_0^h-1) \\ & +\alpha_{2c}P(m-1,1,k_0^{2c}-1)+\alpha_{3h}P(m-1,0,k_0^{3h}-1) \\ & +\alpha_{ch}P(m-1,3,k_0^{ch}-1) \\ & +\alpha_{cch}P(m-2,3,k^{cch}-1)\}\exp\,[i\varphi_0(K_p-K_n)] \\ = {} & (1-\alpha_c-\alpha_{2c}-\alpha_{3c}-\alpha_{ch}-\alpha_{4c}-\alpha_{cch}) \\ & \sum P(m-1,3)\exp\,[i\varphi_0\{-1+(K_p-K_n)\}] \\ & \times\exp\,[+i\varphi_0] \\ & +\alpha_h\sum P(m-1,2,k_0^h-1)\exp[i\varphi_0\{K_p-1-K_n\}] \\ & \times\exp\,[+i\varphi_0] \end{aligned}$$

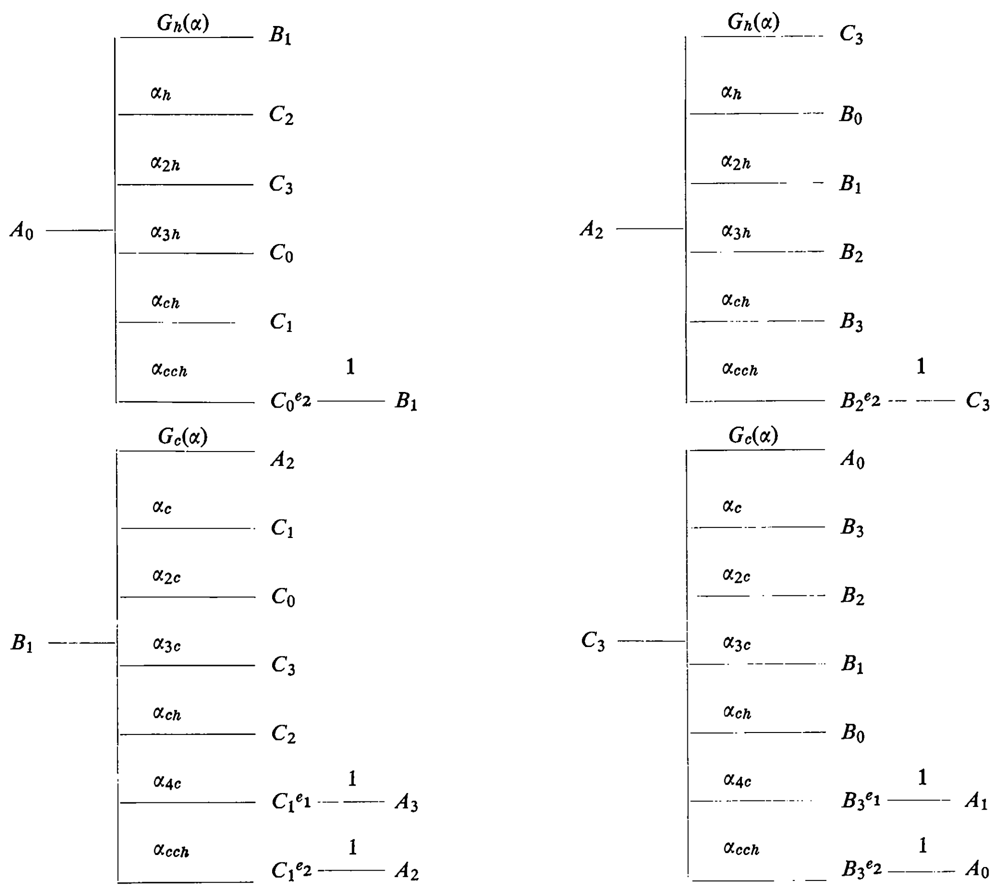

Fig. 1. Probability trees for successive layers $[G_c(\alpha)=1-\alpha_c-\alpha_{2c}-\alpha_{3c}-\alpha_{ch}-\alpha_{4c}-\alpha_{cch};\ G_h(\alpha)=1-\alpha_h-\alpha_{2h}-\alpha_{3h}-\alpha_{ch}-\alpha_{cch}]$.

$$+\alpha_{2c}\sum P(m-1,1,k_0^{2c}-1)\exp[i\varphi_0 \times\{1+(K_p-K_n+1)\}]\exp[+i\varphi_0] +\alpha_{3h}\sum P(m-1,0,k_0^{3h}-1)\exp[i\varphi_0 \times\{K_p-K_n+1\}]\exp[-i\varphi_0] +\alpha_{ch}\sum P(m-1,3,k_0^{ch}-1)\exp[i\varphi_0 \times\{-1+(K_p-1-K_n)\}]\exp[-i\varphi_0] +\alpha_{cch}\sum P(m-2,3,k^{cch}-1)\exp[i\varphi_0 \times\{-1+(K_p-K_n)\}]\exp[+i\varphi_0]\,,\quad m\geq 2\,. \tag{21}$$

Again the summation extends over those values of the k's for which $j=(m-K_i+K_r)$ mod $4=0$ which is equivalent to $(m-1-K_i+K_r)$ mod $4=3$ or $(m-1-K_i+K_r-1)$ mod $4=2$ etc. Utilizing equations (15) and (20) and inserting $\Phi_{m-1}^{A_0}$, $\Phi_{m-2}^{A_0}$ and $J(m,j)$ on the right hand side of equation (21), we have

$$J(m,0)=(1-\alpha_c-\alpha_{2c}-\alpha_{3c}-\alpha_{ch}-\alpha_{4c}-\alpha_{cch})\,\omega \times J(m-1,3)+\alpha_h\omega\, J(m-1,2) +\alpha_{2c}\omega\, J(m-1,1)+\alpha_{3h}\omega^2\, J(m-1,0)+\alpha_{ch}\omega^2 \times J(m-1,3)+\alpha_{cch}\omega\, J(m-2,3)\,,\quad m\geq 2\,, \tag{22}$$

where $\omega=\exp[i\varphi_0]=\exp[2\pi i/3]$. Similarly

$$J(m,1)=(1-\alpha_h-\alpha_{2h}-\alpha_{3h}-\alpha_{ch}-\alpha_{cch})\omega \times J(m-1,0)+\alpha_c\omega\, J(m-1,1) +\alpha_{2h}\omega\, J(m-1,2)+\alpha_{3c}\omega^2\, J(m-1,3)+\alpha_{ch}\omega^2 \times J(m-1,0)+\alpha_{4c}\omega\, J(m-2,3)+\alpha_{cch}\omega \times J(m-2,0)\,,\quad m\geq 2\,. \tag{23}$$

$$J(m,2)=(1-\alpha_c-\alpha_{2c}-\alpha_{3c}-\alpha_{ch}-\alpha_{4c}-\alpha_{cch})\omega^2 \times J(m-1,1)+\alpha_h\omega^2\, J(m-1,0)+\alpha_{2c}\omega^2\, J(m-1,3) +\alpha_{3h}\omega\, J(m-1,2)+\alpha_{ch}\omega\, J(m-1,1)+\alpha_{cch}\omega^2 \times J(m-2,1)\quad m\geq 2\,. \tag{24}$$

$$J(m,3)=(1-\alpha_h-\alpha_{2h}-\alpha_{3h}-\alpha_{ch}-\alpha_{cch})\omega^2 \times J(m-1,2)+\alpha_c\omega^2\, J(m-1,3)+\alpha_{2h}\omega^2\, J(m-1,0) +\alpha_{3c}\omega\, J(m-1,1)+\alpha_{ch}\omega\, J(m-1,2)+\alpha_{4c}\omega^2 \times J(m-2,1)+\alpha_{cch}\omega^2\, J(m-2,2)\,,\quad m\geq 2\,. \tag{25}$$

Let the solution of this system of difference equations be of the form

$$J(m,j)=C_j^{A_0}\,.\,\varrho^m \tag{26}$$

where $C_j^{A_0}$ and ϱ are functions of the α's. Substituting this in equations (22) to (25), we obtain after rearrangement

$$\begin{bmatrix} \varrho^2-\alpha_{3h}\omega^2\varrho & -\alpha_{2c}\omega\varrho & -\alpha_h\omega\varrho & -F_c(\alpha)\omega\varrho-\alpha_{cch}\omega \\ -F_h(\alpha)\omega\varrho-\alpha_{cch}\omega & \varrho^2-\alpha_c\omega\varrho & -\alpha_{2h}\omega\varrho & -\alpha_{3c}\omega^2\varrho-\alpha_{4c}\omega \\ -\alpha_h\omega^2\varrho & -F_c^*(\alpha)\omega^2\varrho-\alpha_{cch}\omega^2 & \varrho^2-\alpha_{3h}\omega\varrho & -\alpha_{2c}\omega^2\varrho \\ -\alpha_{2h}\omega^2\varrho & -\alpha_{3c}\omega\varrho-\alpha_{4c}\omega^2 & -F_h^*(\alpha)\omega^2\varrho-\alpha_{cch}\omega^2 & \varrho^2-\alpha_c\omega^2\varrho \end{bmatrix}\begin{bmatrix} C_0^{A_0} \\ C_1^{A_0} \\ C_2^{A_0} \\ C_3^{A_0}\end{bmatrix}=0 \tag{27}$$

where

$$F_c(\alpha)=1-\alpha_c-\alpha_{2c}-\alpha_{3c}-\alpha_{ch}(1-\omega)-\alpha_{4c}-\alpha_{cch} \tag{28}$$

$$F_h(\alpha)=1-\alpha_h-\alpha_{2h}-\alpha_{3h}-\alpha_{ch}(1-\omega)-\alpha_{cch} \tag{29}$$

and * indicates complex conjugate. For non-trivial values of $C_j^{A_0}$, the determinant of the first matrix must vanish. On simplification, we obtain

$$\varrho^8+(\alpha_c+\alpha_{3h})\varrho^7+(\alpha_c^2-\alpha_h^2+\alpha_{2c}-2\alpha_{2h}-\alpha_{3c}^2+\alpha_{3h}^2)\varrho^6 +[\alpha_h(1-\alpha_h)-2\alpha_{3c}(1-\alpha_{3c})]\varrho^5-[(1-\alpha_c)^2 +(1-\alpha_h)^2-2(\alpha_{2c}+\alpha_{2h})+(1-\alpha_{3c})^2+(1-\alpha_{3h})^2 +\{1-3\alpha_{ch}(1-\alpha_{ch})\}^2-3\alpha_{4c}(1-\alpha_{4c})-(1-\alpha_{cch})^4 -3]\varrho^4-4\alpha_{cch}(1-\alpha_{cch})^3\varrho^3-6\alpha_{cch}^2(1-\alpha_{cch})^2\varrho^2 -4\alpha_{cch}^3(1-\alpha_{cch})\varrho-\alpha_{cch}^4=0\,. \tag{30}$$

It may be pointed out that equation (10) of Jagodzinski (1949), equation (23) of Gevers (1954) and equation (38) of Holloway (1969) can be obtained from the above equation by putting the appropriate α's equal to zero. The roots of equation (30) are

$$\varrho_0=1-\tfrac{3}{4}(\alpha_c+\alpha_h+\alpha_{2c}+\alpha_{3h}+2\alpha_{ch}+\alpha_{4c} \tag{31}$$

$$\varrho_1=-\tfrac{1}{4}(\alpha_c-\alpha_h+2\alpha_{3c}+\alpha_{3h}-4\alpha_{cch}) -i[1-\tfrac{1}{4}(2\alpha_c+2\alpha_h+\alpha_{2c}+4\alpha_{2h}+2\alpha_{3c}+2\alpha_{3h} +6\alpha_{ch}+3\alpha_{4c}+4\alpha_{cch})] \tag{32}$$

$$\varrho_2=-1+\tfrac{1}{4}(\alpha_c+\alpha_h+3\alpha_{2c}+4\alpha_{3c}+\alpha_{3h}+6\alpha_{ch} +3\alpha_{4c}+8\alpha_{cch}) \tag{33}$$

$$\varrho_3=-\tfrac{1}{4}(\alpha_c-\alpha_h+2\alpha_{3c}+\alpha_{3h}-4\alpha_{cch}) +i[1-\tfrac{1}{4}(2\alpha_c+2\alpha_h+\alpha_{2c}+4\alpha_{2h}+2\alpha_{3c}+2\alpha_{3h} +6\alpha_{ch}+3\alpha_{4c}+4\alpha_{cch})] \tag{34}$$

$$\varrho_4=-\alpha_{cch} \tag{35}$$

Since ϱ_1 and ϱ_3 are complex conjugates, we simplify calculations by putting

$$\varrho_1=-R\exp[+i\chi] \tag{36}$$

$$\varrho_3=-R\exp[-i\chi] \tag{37}$$

where

$$R=1-\tfrac{1}{4}(2\alpha_c+2\alpha_h+\alpha_{2c}+4\alpha_{2h}+2\alpha_{3c}+2\alpha_{3h}+6\alpha_{ch} +3\alpha_{4c}+4\alpha_{cch}) \tag{38}$$

$$\chi=\tan^{-1}[4/(\alpha_c-\alpha_h+2\alpha_{3c}+\alpha_{3h}-4\alpha_{cch})]\,. \tag{39}$$

Letting χ_0 be the value of χ for $\alpha_c=\alpha_h=\alpha_{3c}=\alpha_{3h}=\alpha_{cch}=0$, it follows that

$$\chi_0=\tan^{-1}\infty=\frac{\pi}{2} \tag{40}$$

A more convenient expression for χ is as follows;

$$\chi=\chi_0+(\chi-\chi_0)$$
$$=\frac{\pi}{2}-\tfrac{1}{4}(\alpha_c-\alpha_h+2\alpha_{3c}+\alpha_{3h}-4\alpha_{cch}). \quad (41)$$

Equation (30) can be shown to hold for sequences originating with other types of layers as well. Now since

$$\langle\exp[i\Phi_m]\rangle=\sum P(\Phi_m)\exp[i\Phi_m] \quad (42)$$

it follows from equations (20) and (26) that

$$\langle\exp[i\Phi_m]\rangle=\sum_v C_v\varrho_v{}^m\,, \quad m\ge 0 \quad (43)$$

where $P(\Phi_m)$ is the probability of having a phase difference Φ_m in an m layer sequence and

$$C_v=C_v^{A_0}+C_v^{B_1}+C_v^{A_2}+C_v^{C_3}$$
$$+C_v^{C_0^{e2}}+C_v^{C_1^{e2}}+C_v^{B_2^{e2}}+C_v^{B_3^{e2}}+C_v^{C_1^{e1}}+C_v^{B_3^{e1}}$$
$$v=0 \text{ to } 4 \quad (44)$$

The C_v's can be evaluated in three steps as follows: First we find the probability w_j of finding a layer with a particular value of j on passing through an arbitrary region of the crystal. Next we find five initial conditions *i.e.* the values of $\langle\exp[i\Phi_m]\rangle$ for $m=0$ to 4. Finally, the C_v's are found. Consideration of the sequences in Fig. 1 leads to the following relations among the w's

$$w_0=\alpha_{3h}w_0+\alpha_{2c}w_1+\alpha_h w_2$$
$$+(1-\alpha_c-\alpha_{2c}-\alpha_{3c}-\alpha_{4c}-\alpha_{cch})w_3+w_3^{e2} \quad (45)$$

$$w_1=(1-\alpha_h-\alpha_{2h}-\alpha_{3h}-\alpha_{cch})w_0+\alpha_c w_1$$
$$+\alpha_{2h}w_2+\alpha_{3c}w_3+w_3^{e1}+w_0^{e2} \quad (46)$$

$$w_2=\alpha_h w_0+(1-\alpha_c-\alpha_{2c}-\alpha_{3c}-\alpha_{4c}-\alpha_{cch})w_1$$
$$+\alpha_{3h}w_2+\alpha_{2c}w_3+w_1^{e2} \quad (47)$$

$$w_3=\alpha_{2h}w_0+\alpha_{3c}w_1+(1-\alpha_h-\alpha_{2h}-\alpha_{3h}-\alpha_{cch})w_2$$
$$+\alpha_c w_3+w_1^{e1}+w_2^{e2} \quad (48)$$

$$w_1^{e1}=\alpha_{4c}w_1\,; \qquad w_3^{e1}=\alpha_{4c}w_3 \quad (49)\ \&\ (50)$$

$$w_0^{e2}=\alpha_{cch}w_0\,; \qquad w_1^{e2}=\alpha_{cch}w_1 \quad (51)\ \&\ (52)$$

$$w_2^{e2}=\alpha_{cch}w_2\,; \qquad w_3^{e2}=\alpha_{cch}w_3\,. \quad (53)\ \&\ (54)$$

The superscripts e_1 and e_2 refer to extra-ordinary layers due to extrinsic $4c$ and extrinsic cch faults respectively and the subscript for these layers is the same as that of the prior layer. Also

$$w_0+w_1+w_2+w_3+w_1^{e1}+w_3^{e1}+w_0^{e2}$$
$$+w_1^{e2}+w_2^{e2}+w_3^{e2}=1\,. \quad (55)$$

From equations (45) to (55), we get

$$w_0=w_2=\tfrac{1}{4}\left(1-\frac{\alpha_c}{2}+\frac{\alpha_h}{2}-\frac{\alpha_{3c}}{2}+\frac{\alpha_{3h}}{2}-\alpha_{4c}-\alpha_{cch}\right) \quad (56)$$

$$w_1=w_3=\tfrac{1}{4}\left(1+\frac{\alpha_c}{2}-\frac{\alpha_h}{2}+\frac{\alpha_{3c}}{2}-\frac{\alpha_{3h}}{2}-\alpha_{cch}\right) \quad (57)$$

$$w_1^{e1}=w_3^{e1}=\tfrac{1}{4}\alpha_{4c} \quad (58)$$

$$w_0^{e2}=w_1^{e2}=w_2^{e2}=w_3^{e2}=\tfrac{1}{4}\alpha_{cch}\,. \quad (59)$$

Considering all the possible sequences starting with layers of type A_0, B_1, A_2, C_3, C_1^{e1}, B_3^{e1}, C_0^{e2}, C_1^{e2}, B_2^{e2}, B_3^{e2}, one can obtain $\langle\exp[i\Phi_m^{X_j}]\rangle$ in each case (X_j is the layer type) for $m=0$ to 4. Since

$$\langle\exp[i\Phi_m]\rangle=\sum w_j\langle\exp[i\Phi_m^{X_j}]\rangle+\sum w_j^{e1}\langle\exp[i\Phi_m^{X_j^{e1}}]\rangle$$
$$+\sum w_j^{e2}\langle\exp[i\Phi_m^{X_j^{e2}}]\rangle\,, \quad (60)$$

one can find $\langle\exp[i\Phi_m]\rangle$ by substitution for the w's from equations (56) to (59). Thus

$$\langle\exp[i\Phi_0]\rangle=1 \quad (61)$$

$$\langle\exp[i\Phi_1]\rangle=-\tfrac{1}{2} \quad (62)$$

$$\langle\exp[i\Phi_2]\rangle=\tfrac{1}{4}[1-\tfrac{3}{2}(\alpha_c-\alpha_h+2\alpha_{2c}-2\alpha_{2h}+3\alpha_{3c}$$
$$-3\alpha_{3h}+4\alpha_{4c}+2\alpha_{cch})] \quad (63)$$

$$\langle\exp[i\Phi_3]\rangle=-\tfrac{1}{2}[1-\tfrac{3}{2}(\alpha_c+2\alpha_{2c}+3\alpha_{3c}+2\alpha_{ch}+4\alpha_{4c}$$
$$+4\alpha_{cch})] \quad (64)$$

$$\langle\exp[i\Phi_4]\rangle=1-\tfrac{3}{2}(\alpha_c+\alpha_h+\tfrac{3}{2}\alpha_{2c}+\alpha_{2h}+2\alpha_{3c}+\alpha_{3h}$$
$$+4\alpha_{ch}+2\alpha_{4c}+5\alpha_{cch})\,. \quad (65)$$

Substituting from equations (31) to (35) and (61) to (65) in equation (43) and solving for the C's, we obtain

$$C_0=\tfrac{1}{16}-\tfrac{3}{64}(\alpha_c-\alpha_h+4\alpha_{3c}-3\alpha_{3h}+4\alpha_{ch}$$
$$-2\alpha_{4c}+8\alpha_{cch}) \quad (66)$$

$$C_1=\tfrac{3}{16}+\tfrac{3}{32}[(\alpha_c-\alpha_h+\alpha_{3c}-3\alpha_{3h}-2\alpha_{ch}$$
$$+3\alpha_{4c}-6\alpha_{cch})-\frac{i}{2}(\alpha_c+\alpha_h+4\alpha_{2c}+2\alpha_{3c}-3\alpha_{3h}$$
$$+12\alpha_{4c}+12\alpha_{cch})] \quad (67)$$

$$C_2=\tfrac{9}{16}-\tfrac{9}{64}(\alpha_c-\alpha_h-3\alpha_{3h}-4\alpha_{ch}+\tfrac{14}{3}\alpha_{4c}) \quad (68)$$

$$C_3=\tfrac{3}{16}+\tfrac{3}{32}[(\alpha_c-\alpha_h+\alpha_{3c}-3\alpha_{3h}-2\alpha_{ch}+3\alpha_{4c}-6\alpha_{cch})$$
$$+\frac{i}{2}(\alpha_c+\alpha_h+4\alpha_{2c}+2\alpha_{3c}-3\alpha_{3h}+12\alpha_{4c}+12\alpha_{cch})] \quad (69)$$

$$C_4=-\tfrac{3}{2}\alpha_{cch}\,. \quad (71)$$

Introducing C_r and C_i through

$$C_r=\tfrac{8}{3}(C_1+C_3)=1+\tfrac{1}{2}(\alpha_c-\alpha_h+\alpha_{3c}-3\alpha_{3h}-2\alpha_{ch}$$
$$+3\alpha_{4c}-6\alpha_{cch}) \quad (71)$$

$$C_i=\tfrac{8}{3i}(-C_1+C_3)=\tfrac{1}{4}(\alpha_c+\alpha_h+4\alpha_{2c}+2\alpha_{3c}-3\alpha_{3h}$$
$$+12\alpha_{4c}+12\alpha_{cch})\,, \quad (72)$$

we can express C_1 and C_3 as

$$C_1=\tfrac{3}{16}\,(C_r-iC_i) \tag{73}$$

$$C_3=\tfrac{3}{16}\,(C_r+iC_i)\,. \tag{74}$$

Substituting from equations (31), (33), (35), (36), (37), (73), (74) in equation (43) and simplifying, we have

$$\langle\exp\,[i\Phi_m]\rangle=C_0\varrho_0{}^m+\tfrac{3}{8}\,(C_r\cos m\chi+C_i\sin m\chi)\times(-R)^m+C_2\varrho_2^m+C_4\varrho_4^m \quad m\geq 0 \tag{75}$$

Proceeding as above, we have for negative values of m

$$\langle\exp\,[i\Phi_m]\rangle=C_0\varrho_0{}^{|m|}+\tfrac{3}{8}\,(C_r\cos m\chi+C_i\sin |m|\chi)\,(-R)^{|m|}+C_2\varrho_2{}^{|m|}+C_4\varrho_4^{|m|} \quad m\leq 0 \tag{76}$$

Substituting from equations (75) and (76) in equation (3), we obtain for the diffracted intensity,

$$\begin{aligned}I(h_3)=&\,C_0\psi^2\sum_{m=-\infty}^{\infty}\varrho_0^{|m|}\cos\left[\frac{m\pi h_3}{2}\right]\\&+\tfrac{3}{8}C_r\psi^2\sum_{m=-\infty}^{\infty}(-R)^{|m|}\,[\cos m\chi+C_i\sin|m|\chi]\\&\times\cos\left[\frac{m\pi h_3}{2}\right]\\&+C_2\psi^2\sum_{m=-\infty}^{\infty}\varrho_2^{|m|}\cos\left[\frac{m\pi h_3}{2}\right]\\&+C_4\psi^2\sum_{m=-\infty}^{\infty}\varrho_4^{|m|}\cos\left[\frac{m\pi h_3}{2}\right]\end{aligned} \tag{77}$$

where we have expanded $\exp\,[im\pi h_3/2]$ into cosine and sine components so that terms involving $\sin\,[m\pi h_3/2]$ cancel in pairs. Utilizing the relations for $\cos A\cos B$ and $\sin A\cos B$ and expanding the second term in equation (77), the expression for the intensity reduces to

$$\begin{aligned}I(h_3)=&\,C_0\psi^2\sum\varrho_0^{|m|}\cos\left[\frac{m\pi h_3}{2}\right]\\&+\tfrac{3}{16}C_r\psi^2\sum R^{|m|}\left\{\cos\left[m\left(\frac{\pi h_3}{2}+\chi-\pi\right)\right]\right.\\&\left.+C_i\sin\left[|m|\left(\frac{\pi h_3}{2}+\chi-\pi\right)\right]\right\}\\&+C_2\psi^2\sum(-\varrho_2)^{|m|}\cos\left[m\left(\frac{\pi h_3}{2}-\pi\right)\right]\\&+\tfrac{3}{16}C_r\psi^2\sum R^{|m|}\left\{\cos\left[m\left(\frac{\pi h_3}{2}-\chi+\pi\right)\right]\right.\\&\left.-C_i\sin\left[|m|\left(\frac{\pi h_3}{2}-\chi+\pi\right)\right]\right\}\\&+C_4\psi^2\sum(-\varrho_4)^{|m|}\cos\left[m\left(\frac{\pi h_3}{2}-\pi\right)\right].\end{aligned} \tag{78}$$

Carrying out the summations, we get

$$\begin{aligned}I(h_3)=&\,\psi^2\frac{C_0\,(1-\varrho_0^2)}{1-2\varrho_0\cos\,[\pi h_3/2]+\varrho_0^2}\\&+\tfrac{3}{16}\psi^2\frac{C_r\,(1+2C_i\,R\sin\,[\pi h_3/2+\chi-\pi]-R^2)}{1-2R\cos\,[\pi h_3/2+\chi-\pi]+R^2}\\&+\psi^2\frac{C_2\,(1-\varrho_2^2)}{1+2\varrho_2\cos\,[\pi h_3/2-\pi]+\varrho_2^2}\\&+\psi^2\frac{C_4(1-\varrho_4^2)}{1+2\varrho_4\cos\,[\pi h_3/2-\pi]+\varrho_4^2}\\&+\tfrac{3}{16}\psi^2\frac{C_r\,(1-2C_i\,R\sin\,[\pi h_3/2-\chi+\pi]-R^2)}{1-2R\cos\,[\pi h_3/2-\chi+\pi]+R^2}\,.\end{aligned} \tag{79}$$

Description of diffraction effects

For reflexions with $H-K=0$ mod 3, sharp peaks corresponding to $L=0$ mod 4 occur. For reflexions with $H-K\neq 0$ mod 3, the first, second, third and fourth, fifth terms on the right hand side of equation (79) give rise to broadened peaks corresponding to $L=0$, 1, 2, 3 mod 4. The fourth term gives rise to a rather diffuse peak which vanishes for $\alpha_{cch}=0$. In general, there are changes in integrated intensity and peak broadening for all reflexions. In addition, reflexions with $L=\pm 1$ mod 4 exhibit peak shift and peak asymmetry. These can be utilized for estimating fault probabilities. Quantitative expressions for the profile characteristics mentioned above are given in the following.

Determination of fault parameters from peak integrated intensity

The integrated intensities T_0, T_1, T_2, T_3 for reflexions with $L=0$, 1, 2, 3 mod 4 can be obtained by integrating separately the terms (considering the third and fourth terms together) on the right hand side of equation (79) and are:

$$T_0=\frac{\psi^2}{4}\,[1-\tfrac{3}{4}\,(\alpha_c-\alpha_h+4\alpha_{3c}-3\alpha_{3h}+4\alpha_{ch}-2\alpha_{4c}+8\alpha_{cch})] \tag{80}$$

$$T_1=\frac{3\psi^2}{4}\,[1+\tfrac{1}{2}\,(\alpha_c-\alpha_h+\alpha_{3c}-3\alpha_{3h}-2\alpha_{ch}+3\alpha_{4c}-6\alpha_{cch})] \tag{81}$$

$$T_2=\frac{9\psi^2}{4}\,[1-\tfrac{1}{4}\,(\alpha_c-\alpha_h-3\alpha_{3h}-4\alpha_{ch}+\tfrac{14}{3}\alpha_{4c}-\tfrac{32}{3}\alpha_{cch})] \tag{82}$$

$$T_3=\frac{3\psi^2}{4}\,[1+\tfrac{1}{2}\,(\alpha_c-\alpha_h+\alpha_{3c}-3\alpha_{3h}-2\alpha_{ch}+3\alpha_{4c}-6\alpha_{cch})]\,. \tag{83}$$

For all α's equal to 0, T_0, T_1, T_2, T_3 reduce to $\psi^2/4$, $3\psi^2/4$, $9\psi^2/4$, $3\psi^2/4$ respectively, characteristic of the perfect d.h.c.p. structure. For non-vanishing values of the α's, there are changes in the integrated intensities, However, in practice, it is easier to measure fractional changes in the ratios

$$R_1 = T_1/T_0 \tag{84}$$

and

$$R_2 = T_2/T_0\,. \tag{85}$$

For the perfect structure $R_1=3$ and $R_2=9$. From equations (80) to (83), the fractional changes in R_1 and R_2 are given by

$$\frac{\Delta R_1}{R_1} = \tfrac{5}{4}\alpha_c - \tfrac{5}{4}\alpha_h + \tfrac{7}{2}\alpha_{3c} - \tfrac{15}{4}\alpha_{3h} + 2\alpha_{ch} + 3\alpha_{cch} \tag{86}$$

$$\frac{\Delta R_2}{R_2} = \tfrac{1}{2}\alpha_c - \tfrac{1}{2}\alpha_h + 3\alpha_{3c} - \tfrac{3}{2}\alpha_{3h} + 4\alpha_{ch} + \tfrac{1}{3}\alpha_{4c} + 12\alpha_{cch}\,. \tag{87}$$

Thus from equations (86) and (87), we have estimates of two compound fault parameters.

Determination of fault parameters from peak shifts

For reflexions with $L=\pm 1$ mod 4, the peak shifts are given by

$$\Delta h_3 = \pm \frac{1}{2\pi}(\alpha_c - \alpha_h + 2\alpha_{3c} + \alpha_{3h} - 4\alpha_{cch})\,, \qquad L=\pm 1 \text{ mod } 4 \tag{88}$$

Converting to 2θ coordinates we get for the peak shifts

$$\Delta(2\theta)^\circ = \pm \frac{180}{\pi^2}\cdot\frac{|L|d^2}{c^2}\tan\theta\,(\alpha_c - \alpha_h + 2\alpha_{3c} + \alpha_{3h} - 4\alpha_{cch})\,, \quad L=\pm 1 \text{ mod } 4 \tag{89}$$

Thus measurement of $\Delta(2\theta)^\circ$ leads to an estimate of a third compound fault parameter. We may add that experimental errors can be minimized by using a pair of neighbouring reflexions having opposite peak shifts and measuring the change in separation of the two peaks.

Determination of fault probabilities from peak broadening

1. *Integral breadth analysis*

A simple measure of the peak broadening is the integral breadth which is the ratio of the peak integrated intensity and the peak maximum. Dividing equations (80) to (83) by the respective peak maxima, we get for the integral breadths β_j for reflexions with $L=j$ mod 4:

$$\beta_0 = \tfrac{3}{2}(\alpha_c + \alpha_h + \alpha_{2c} + \alpha_{3h} + 2\alpha_{ch} + \alpha_{4c})\,, \qquad L=0 \text{ mod } 4 \tag{90}$$

$$\beta_1 = \beta_3 = (\alpha_c + \alpha_h + \tfrac{1}{2}\alpha_{2c} + 2\alpha_{2h} + \alpha_{3c} + \alpha_{3h} + 3\alpha_{ch} + \tfrac{3}{2}\alpha_{4c} + 2\alpha_{cch})\,, \qquad L=\pm 1 \text{ mod } 4 \tag{91}$$

$$\beta_2 = \tfrac{1}{2}(\alpha_c + \alpha_h + 3\alpha_{2c} + 4\alpha_{3c} + \alpha_{3h} + 6\alpha_{ch} + 3\alpha_{4c} + 8\alpha_{cch})\,, \qquad L=2 \text{ mod } 4 \tag{92}$$

Thus measurement of β_0, β_1 or β_3 and β_2 leads to estimates of three more compound fault parameters. In order to convert the integral breadths to 2θ coordinates we need multiply the expressions (90) to (92) by $(\lambda/\cos\theta)\,(|L|\,d/c^2)$.

2. *Fourier analysis*

Another measure of broadening is the initial slope of the Fourier coefficients of a peak. Following Warren (1959), we convert equation (78) to the observable power distribution in a powder pattern reflexion. Considering each reflexion as $00l$ in terms of orthorhombic axes a_3' and its reciprocal b_3', we express the powder pattern peak shapes $P'_{2\theta}$ by four Fourier series in which the Fourier coefficients are correctly expressed only for small values of n:

(i) $L=0$ mod 4

$$P'_{2\theta} = \frac{GC_0}{b_3'}\sum_n \left[1 - \frac{|n|}{b_3'}\cdot\frac{|L|d}{c^2}\cdot 3\,(\alpha_c + \alpha_h + \alpha_{2c} + \alpha_{3h} + 2\alpha_{ch} + \alpha_{4c})\right] \times \cos 2\pi n\,(h_3' - l')\,. \tag{93}$$

(ii) $L=1$ mod 4

$$P'_{2\theta} = \tfrac{3}{16}\frac{GC_r}{b_3'}\sum_n \left[1 - \frac{|n|}{b_3'}\,\frac{|L|d}{c^2}\,2\,(\alpha_c + \alpha_h + \tfrac{1}{2}\alpha_{2c} + 2\alpha_{2h} + \alpha_{3c} + \alpha_{3h} + \tfrac{3}{2}\alpha_{4c} + 2\alpha_{cch})\right] \times [\cos 2\pi n\,(h_3' - l' - \delta) + C_t \sin 2\pi|n|\,(h_3' - l' - \delta)]\,. \tag{94}$$

(iii) $L=2$ mod 4

$$P'_{2\theta} = \frac{GC_2}{b_3'}\sum_n \left[1 - \frac{|n|}{b_3'}\,\frac{|L|d}{c^2}\,(\alpha_c + \alpha_h + 3\alpha_{2c} + 4\alpha_{3c} + \alpha_{3h} + 6\alpha_{ch} + 3\alpha_{4c} + 8\alpha_{cch})\right] \times \cos 2\pi n\,(h_3' - l')\,. \tag{95}$$

(iv) $L=3$ mod 4

$$P'_{2\theta} = \tfrac{3}{16}\frac{GC_r}{b_3'}\sum_n \left[1 - \frac{|n|}{b_3'}\cdot\frac{|L|d}{c^2}\,2(\alpha_c + \alpha_h + \tfrac{1}{2}\alpha_{2c} + 2\alpha_{2h} + \alpha_{3c} + \alpha_{3h} + 3\alpha_{ch} + \tfrac{3}{2}\alpha_{4c} + 2\alpha_{cch})\right] \times [\cos 2\pi n\,(h_3' - l' + \delta) - C_t \sin 2\pi\,|n|\,(h_3' - l' + \delta)] \tag{96}$$

where

$$\delta = \frac{1}{b_3'}\cdot\frac{|L|d}{c^2}\cdot\frac{1}{2\pi}(\alpha_c - \alpha_h + 2\alpha_{3c} + \alpha_{3h} - 4\alpha_{cch})\,. \tag{97}$$

Let the Fourier cosine and sine coefficients be represented by A_n and B_n respectively. Expressing the coefficients in terms of a real length $L_0 = na_3' = n/b_3'$, we get

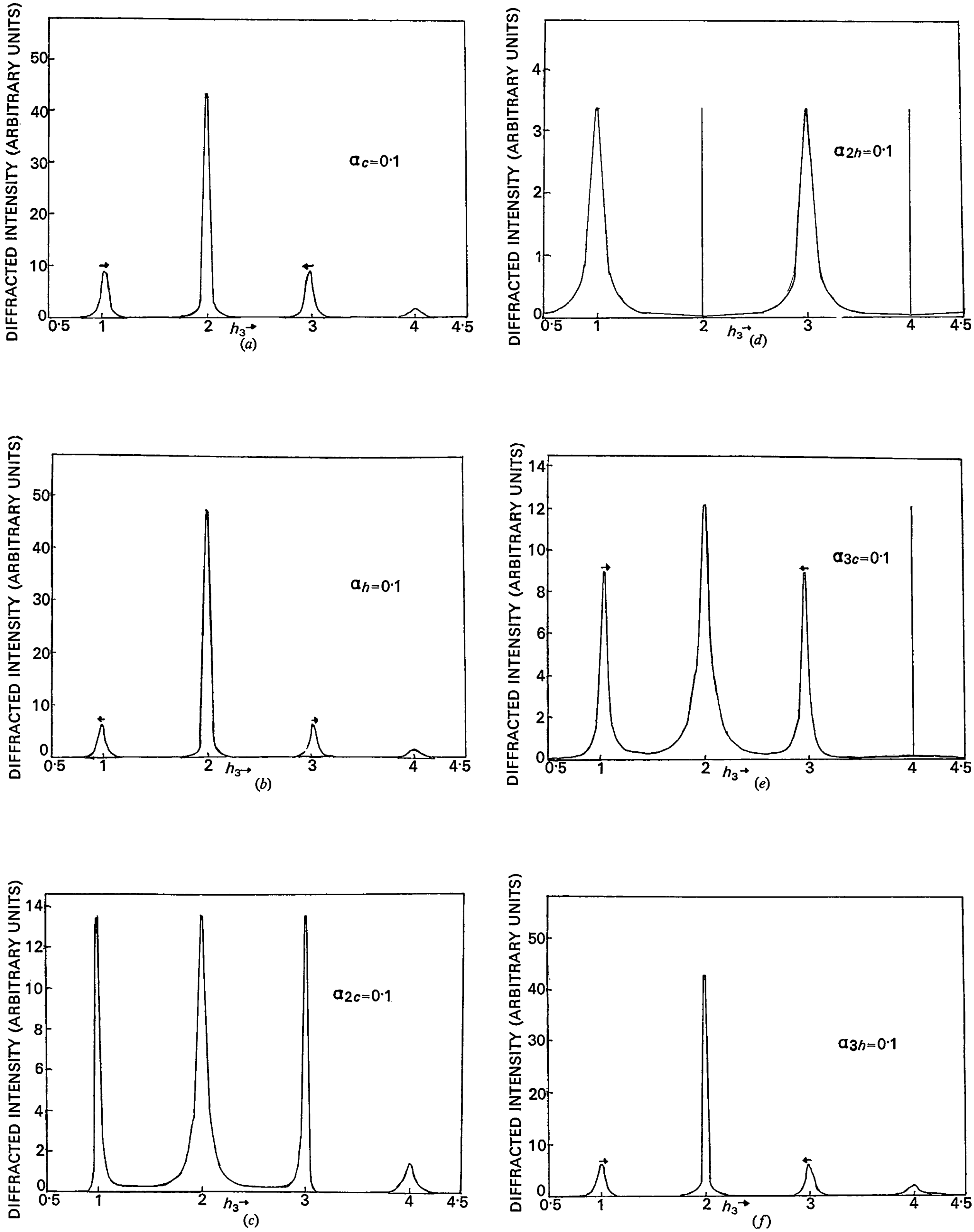

Fig. 2. Diffracted intensity as a function of h_3: (*a*) intrinsic *c* faults ($\alpha_c = 0{\cdot}1$), (*b*) intrinsic *h* faults ($\alpha_h = 0{\cdot}1$), (*c*) intrinsic 2*c* faults ($\alpha_{2c} = 0{\cdot}1$), (*d*) intrinsic 2*h* faults ($\alpha_{2h} = 0{\cdot}1$), (*e*) intrinsic 3*c* faults ($\alpha_{3c} = 0{\cdot}1$), (*f*) intrinsic 3*h* faults ($\alpha_{3h} = 0{\cdot}1$).

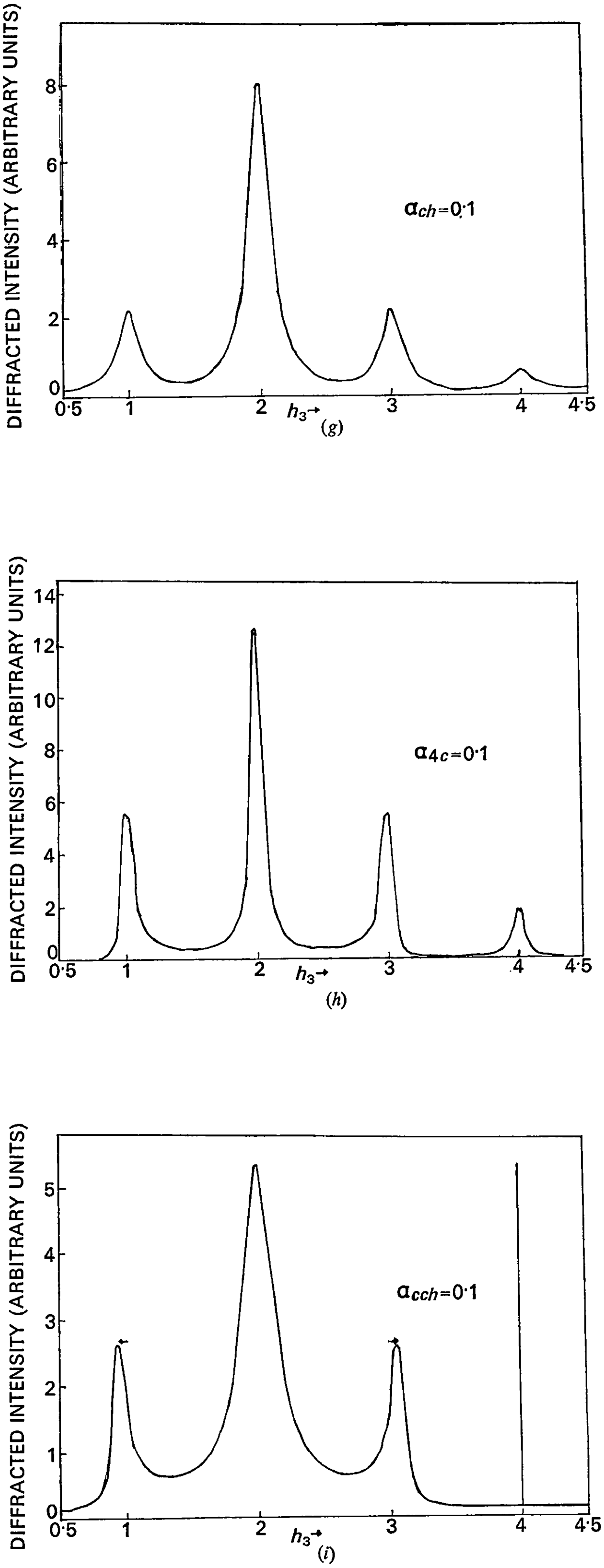

Fig. 2 (*cont.*). (*g*) intrinsic *ch* faults ($\alpha_{ch}=0{\cdot}1$), (*h*) extrinsic 4*c* faults ($\alpha_{4c}=0{\cdot}1$), (*i*) extrinsic *cch* faults ($\alpha_{cch}=0{\cdot}1$).

$$-\left(\frac{\mathrm{d}A_{L0}}{\mathrm{d}L_0}\right)_0=\frac{|L|d}{c^2}3\ (\alpha_c+\alpha_h+\alpha_{2c}+\alpha_{3h}+2\alpha_{ch}+\alpha_{4c})\ ,\ L=0 \bmod 4 \quad (98)$$

$$-\left(\frac{\mathrm{d}A_{L0}}{\mathrm{d}L_0}\right)_0=\frac{|L|d}{c^2}2\ (\alpha_c+\alpha_h+\tfrac{1}{2}\alpha_{2c}+2\alpha_{2h}+\alpha_{3c}+\alpha_{3h}+3\alpha_{ch}+\tfrac{3}{2}\alpha_{4c}+2\alpha_{cch})\ ,\quad L=\pm 1 \bmod 4 \quad (99)$$

$$-\left(\frac{\mathrm{d}A_{L0}}{\mathrm{d}L_0}\right)_0=\frac{|L|d}{c^2}(\alpha_c+\alpha_h+3\alpha_{2c}+4\alpha_{3c}+\alpha_{3h}+6\alpha_{ch}+3\alpha_{4c}+8\alpha_{cch})\ ,\ L=2 \bmod 4 \quad (100)$$

Thus, measurement of the initial slope from plots of A_{L0} against L_0 leads to estimates of the same compound fault parameters as obtained from integral breadth analysis.

Determination of fault probabilities from peak asymmetry

1. *Fourier analysis*

A simple measure of asymmetry is the ratio B_n/A_n of the Fourier sine and cosine coefficients. Since $B_n=0$ for reflexions with $L=0$ and 2 mod 4, these reflexions are symmetric. For reflexions with $L=\pm 1$ mod 4, we obtain from equations (94) and (96)

$$\frac{B_n}{A_n}=\pm\tfrac{1}{4}\ (\alpha_c+\alpha_h+4\alpha_{2c}+2\alpha_{3c}-3\alpha_{3h}+12\alpha_{4c}+12\alpha_{cch})\ ,\ L=\pm 1 \bmod 4\ . \quad (101)$$

There are, however, serious limitations in the accurate measurement of the sine coefficients.

2. *Centroid shift*

Another measure of asymmetry is the shift of the centroid of a profile from its peak maximum position. Following Cohen & Wagner (1962), this is given by

$$(\Delta h_3)_{\text{centroid}}=-\frac{1}{2\pi}\sum_{n\neq 0}(-1)^n\frac{B_n}{n}\ . \quad (102)$$

Substituting from equations (94) and (96), converting to 2θ coordinates and simplifying, we have

$$\Delta(2\theta)^\circ{}_{\text{centroid}}=\pm\frac{90\ \ln 2}{\pi^2}\tan\theta\ (\alpha_c+\alpha_h+4\alpha_{2c}+2\alpha_{3c}-3\alpha_{3h}+12\alpha_{4c}+12\alpha_{cch})\ ,\ L=\pm 1 \bmod 4\ . \quad (103)$$

Thus, measurement of asymmetry leads to an estimate of a seventh compound fault parameter.

Discussion of results

Independent estimates of seven compound fault parameters obtained from measurements of the profile characteristics mentioned above are summarized here:

$$\begin{bmatrix} \Delta R_1/R_1 \\ \Delta R_2/R_2 \\ 2\pi\Delta h_3 \\ \beta_0 \\ \beta_1 \\ \beta_2 \\ B_n/A_n \end{bmatrix} = \begin{bmatrix} +\frac{5}{4} & -\frac{5}{4} & 0 & 0 & +\frac{7}{2} & -\frac{15}{4} & +2 & 0 & 0 \\ +\frac{1}{2} & -\frac{1}{2} & 0 & 0 & +3 & -\frac{3}{2} & +4 & +\frac{1}{3} & +\frac{8}{3} \\ +1 & -1 & 0 & 0 & +2 & +1 & 0 & 0 & -4 \\ +\frac{3}{2} & +\frac{3}{2} & +\frac{3}{2} & 0 & 0 & +\frac{3}{2} & +2 & +1 & 0 \\ +1 & +1 & +\frac{1}{2} & +2 & +1 & +1 & +3 & +\frac{3}{2} & +2 \\ +\frac{1}{2} & +\frac{1}{2} & +\frac{3}{2} & 0 & +2 & +\frac{1}{2} & +3 & +\frac{3}{2} & +4 \\ +\frac{1}{4} & +\frac{1}{4} & +1 & 0 & +\frac{1}{2} & -\frac{3}{4} & 0 & +3 & +3 \end{bmatrix} \begin{bmatrix} \alpha_c \\ \alpha_h \\ \alpha_{2c} \\ \alpha_{2h} \\ \alpha_{3c} \\ \alpha_{3h} \\ \alpha_{ch} \\ \alpha_{4c} \\ \alpha_{cch} \end{bmatrix} \tag{104}$$

Obviously, all the nine fault probabilities cannot be evaluated. In fact, only seven parameters are sufficient to satisfy any observed data. The choice of parameters is guided to some extent by the theoretical restriction that $0 \le \alpha \le 1$. In practice, we can omit from consideration two faults with the highest energies. These energies are based on the energies of transformation to the f.c.c. (γ_{TC}) and h.c.p. (γ_{TH}) structures. Thus three cases need to be considered $\gamma_{TC} \gg \gamma_{TH}$, $\gamma_{TC} \simeq \gamma_{TH}$ and $\gamma_{TC} \ll \gamma_{TH}$. The faults having the highest energies in the three cases are respectively (1) intrinsic $3c$ and extrinsic $4c$, (2) intrinsic $3h$ and extrinsic $4c$, (3) intrinsic $2h$ and intrinsic $3h$. Omitting the pair of faults with highest energy in any given case, one can solve equation (104) to obtain the remaining α's.

We may point out that broadening and displacement of peaks can be understood by simple geometrical considerations (Lele & Rama Rao, 1970*a*, *b*).

The variation of intensity in reciprocal space for all the faults is illustrated in Fig. 2 for a particular value of the fault probability. The different diffraction effects of the nine faults are clearly brought out here.

In practical situations small domains and distortions within the specimen in addition to stacking faults are likely to be present. The effects of distortion can be separated by the multiple order technique of Warren & Averbach (1952) while the effects of domain size may be separated by considering reflexions with $H-K=0$ mod 3 which are not affected by faults. Effects of violation of assumptions (3) to (6) are not known.

Several rare-earth metals and their alloys are known to exhibit the d.h.c.p. structure (Speight, Harris & Raynor, 1968). Further, several noble metal alloy systems exhibit d.h.c.p. electron phases intermediate in composition to the f.c.c. solid solution and the h.c.p. ζ phase and some alloys of titanium ($TiNi_3$ and $TiPd_2$) also crystallize in this structure (Schubert, 1964). This four-layer structure has been observed by subjecting some metals and alloys to high pressure (Jayaraman, 1965; Perez-Albuerne, Clendenen, Lynch & Drickamer, 1966). Interesting information regarding propensity to faulting on deformation and/or transformation of these substances can be obtained by powder diffractometer studies. Preliminary studies on plastically deformed $TiNi_3$ by Anantharaman & Vasudevan (1970) indicate the predominance of intrinsic *ch* faults. Further studies on $TiNi_3$ as also $TiPd_2$ are presently in progress.

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