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A General Theory for the Diffraction Line Profiles of H.c.p. and F.c.c. Polycrystals Containing Stacking Faults

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A general theory is proposed for the diffraction line profiles of powders of close-packed crystals containing stacking faults. It covers two theories; one is the Gevers theory which combines the 'growth fault' with s (*Reichweite*) $=2$ and the '*single* deformation fault' in h.c.p., and the other the theory of the '*extended* growth fault' with $s=2$. The anomalies in the line profiles of nearly h.c.p. and nearly f.c.c. powders, *i. e.* peak displacement, broadening, and asymmetry, are expressed as functions of stacking fault probabilities. The conclusion is as follows. Although the Gevers–Warren theory, which is being widely used for interpreting experimental results, is useful from the practical point of view, the fault probabilities obtained by use of this theory should only be taken as very rough estimates.

Introduction

Close-packed crystals, such as h.c.p. and f.c.c. crystals, generally contain many types of faults in stacking of the close-packed atomic layers. A classification of those types of stacking faults that have so far been dealt with is presented in Table 1. To the right of each type of stacking fault are listed the types which are included in it as special cases. Throughout the present paper, each of the Roman numerals (I) to (X) represents not only a type of stacking fault, but also the crystal structure containing the faults concerned, and the relevant diffraction theory.

'Growth faults' are kinds of stacking faults that occur during crystal growth by successive stackings of the unit-layers (Paterson, 1952; Barrett, 1952). For these a certain stacking sequence is equivalent to its *twinned* counterpart; *e.g.* the sequences *AB*, *ABC*, and *ABA* are equivalent to *AC*, *ACB*, and *ACA*, respectively, where *A*, *B*, and *C* are the usual symbols for the three possible lateral positions of the unit-layers. In Table 1 'growth faults' are classified with respect to their 'Reichweite' s (Jagodzinski, 1949*a*), *i.e.* the number of unit-layers preceding a given layer which are effective in determining the position of the given layer. In order to keep a crystal close-packed, $s \geq 1$ is necessary. No variable fault probabilities are associated with the 'growth fault' with $s=1$ (I), and this is the most random case of close-packing. Variable fault probabilities, 2^{s-2} in number, are associated with the cases of $s \geq 2$. Two extreme cases involved in the Wilson theory (II) are the h.c.p. and f.c.c. structures.

For surveying various cases involved in the theory of a type of stacking fault, it is convenient to make up a space based on the relevant fault probabilities. The probability space for the Jagodzinski theory (III) is illustrated in Fig. 12 of a previous paper by the present author (Sato, 1962).

When the above equivalence of a stacking sequence to its *twinned* counterpart is abandoned, new types of stacking faults result. They are referred to as 'extended growth faults'. The necessity of this abandonment in the theory of stacking faults has been pointed out by Kakinoki, Komura & Hiziya (1955) and Kakinoki (1961, 1965, 1967), and experimental evidence favouring it has been presented by Nishiyama, Kakinoki &

Table 1. *Various types of stacking faults in close-packed crystals*

Growth faults		(I)	$s=1$: most random[1,2]	
		(II)	$s=2$: WILSON[3,4]	(I)
		(III)	$s=3$: JAGODZINSKI[1,5,6]	(I) (II)
Extended growth faults		(IV)	$s=1$: PATERSON[7]	(I)
		(V)	$s=2$: KAKINOKI[8,9]	(I) (II) (IV)
		(VI)	$s=3$: KAKINOKI[8,9]	(I) (II) (III) (IV) (V)
Deformation faults	in h.c.p.	(VII)	single: CHRISTIAN[10]	(I)
		(VIII)	double: SATO[11]	
	in f.c.c.	(IV)	single: PATERSON[7]	(I)
		(IX)	double: JOHNSON[12,13]	
		(X)	triple: SATO[1]	

(1) Jagodzinski (1949*a*), (2) Guinier (1956), (3) Wilson (1942), (4) Hendricks & Teller (1942), (5) Jagodzinski (1949*b*), (6) Jagodzinski (1949*c*), (7) Paterson (1952), (8) Kakinoki (1965), (9) Kakinoki (1967), (10) Christian (1954), (11) Sato (1969), (12) Johnson (1963), (13) Warren (1963), (14) Sato (1966*a*).

Kajiwara (1965) from a martensitic Cu–Al alloy. For 'extended growth faults' the necessary fault probabilities are 2^{s-1} in number. The probability space for the $s=2$ theory is illustrated by Kakinoki (1965) (see Fig. 2 below).

On the other hand, a 'deformation fault' arises if a shearing force parallel to the stacking layers gives rise to a translation of one half of a close-packed crystal relative to the other half (Paterson, 1952; Barrett, 1952). In view of the fact that the 'Reichweiten' for 'deformation faults' can be invariably thought of as unity in a mathematical formalism, they are classified in Table 1 with respect to their original stacking pattern; two simple cases are the Christian theory (VII) for h.c.p. and the Paterson theory (IV) for f.c.c. In addition, '*multiple* deformation faults' should be dealt with. The '*single*' (IV) and '*double*' (IX) deformation faults in f.c.c. are referred to also as the '*intrinsic*' and '*extrinsic*' stacking faults, respectively (*e.g.* Barrett & Massalski, 1966). It is remarkable that all the layers outside a '*double*' deformation fault in h.c.p. (VIII) or a '*triple*' deformation fault in f.c.c. (X) maintain the original regular positions (Sato, 1966*a*, 1969). If the fault probability for any type of 'deformation fault', invariably one in number, approaches unity, the structure tends invariably to the twin of the original structure.

As is seen in Table 1, the Paterson case (IV) can be understood in two ways: it is either the 'extended growth fault' with $s=1$ or the 'single deformation fault' in f.c.c.

The terms 'growth' and 'deformation' used above characterize only the geometry of stacking sequences; they should not be understood as suggesting any actual physical process giving rise to the fault. For instance, a 'growth fault' can occur not only during growth, but also during deformation, and also during other processes, such as transformation. This remark should be borne in mind in the physical interpretation of the fault probabilities obtained from experiments.

The Gevers theory (II + VII) and the $s=2$ theory (V)

Gevers (1954) combined the Wilson theory (II) and the Christian theory (VII); for the h.c.p. structures containing growth faults ($s=2$) and deformation faults (single) he obtained a formula for the intensity distribution in reciprocal space by use of the difference equation method (Wilson, 1942, 1962). His result was confirmed by Kakinoki (1965, 1969) by use of the matrix method (Hendricks & Teller, 1942; Kakinoki & Komura, 1952, 1954*a*,*b*, 1965; Kakinoki, 1961, 1965, 1966*a*, 1967).

The probability space for the Gevers theory (II + VII) is shown in Fig. 1, where α and β are growth and deformation fault probabilities in h.c.p., respectively. The space is referred to as the Gevers square. The left lower corner (origin) represents the original h.c.p., and the right lower one the f.c.c., a half of which is the twin of the other half (f.c.c. $\pm$). The terms positive (+) and negative (−) denote the sequences $A \rightarrow B \rightarrow C \rightarrow A$ and $A \rightarrow C \rightarrow B \rightarrow A$, respectively (*International Tables for X-ray Crystallography*, 1959). Since any point in the upper side invariably represents the twin of the structure represented by the corresponding point in the lower side, the meanings of the other two corners are as indicated. The diffraction theory for the lower, upper, or left-hand side is the Wilson theory (II) or the Christian theory (VII). That for the right-hand side is the Paterson theory, but with the condition that a certain stacking sequence and its *twinned* counterpart occur invariably with a common probability. This condition leads to $W_-=0{\cdot}5$, where W_- is the fraction of two-layer negative sequences [see equation (6) below]. The Paterson theory modified in this way is denoted by Paterson* (IV*). In the two lines, $\alpha=0{\cdot}5$ and $\beta=0{\cdot}5$, the structure turns into the most random close-packed one (I). The intensity distributions in reciprocal space at many points in the Gevers square have been numerically calculated by Kakinoki (1966*b*).

For powders of nearly h.c.p. and nearly f.c.c. structures, where growth and deformation faults are both rare, Warren (1959) has obtained formulae expressing the anomalies in the diffraction line profiles, *i.e.* peak displacement, broadening, and asymmetry [see also Anantharaman & Christian (1956) and Wagner (1957)].† Although, according to Kakinoki (1965, 1969), Warren's derivation contains some inadequate reasoning, the formulae obtained are correct in the vicinities of the four corners of the Gevers square. By his formulae, growth and deformation fault probabilities can be determined separately.

Although the Gevers theory (II + VII), which leads to Warren's formulae for polycrystal cases of low fault

† Note that Warren (1959) uses α and β for deformation and growth fault probabilities respectively, in either the h.c.p. or f.c.c. structure.

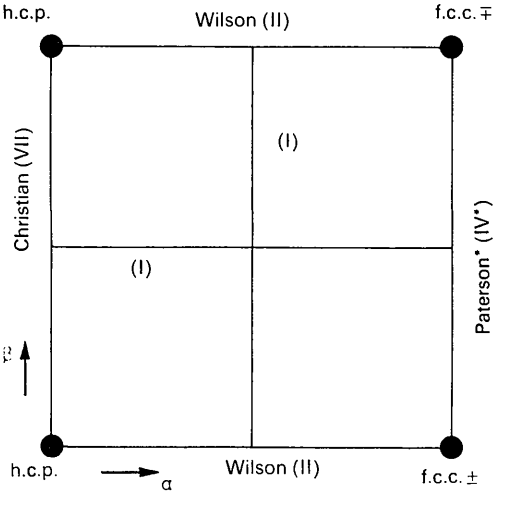

Fig. 1. The Gevers square for (II + VII).

probabilities, is concerned with single-crystals, it invariably postulates $W_{-}=0{\cdot}5$; thus W_{-} of a f.c.c.+ crystal containing stacking faults must be 0·5, however rare the faults may be. In order to avoid such an unreasonable situation, it is necessary to replace this theory with a new one, where W_{-} is not confined to 0·5. Out of many possibilities for such a theory, the simplest one may be the theory of the extended growth fault with $s=2$ (V) (Kakinoki, 1965).

The probability space for this theory, *i.e.* the $s=2$ square, is shown in Fig. 2, where two extended growth fault probabilities, α_1 and α_2, are so defined as to make the structure more positive and negative, respectively, as their values increase. The right-hand side (thick line) represents f.c.c.+, and the upper side (thick broken line) f.c.c.−. W_{-} at the right upper corner depends on the way along which the corner is approached; it becomes equal to 0·5 if the corner is approached along the diagonal. For a diagonal, $\alpha_1=\alpha_2$, the theory reduces to the Wilson theory (II), and for the other, $\alpha_1+\alpha_2=1$, to the Paterson theory (IV). At the centre, $\alpha_1=\alpha_2=0{\cdot}5$, the theory reduces again to that regarding the most random structure (I). The intensity distributions in reciprocal space at many points in the $s=2$ square have been numerically calculated by Kakinoki (1966*b*), for both single and polycrystal cases.

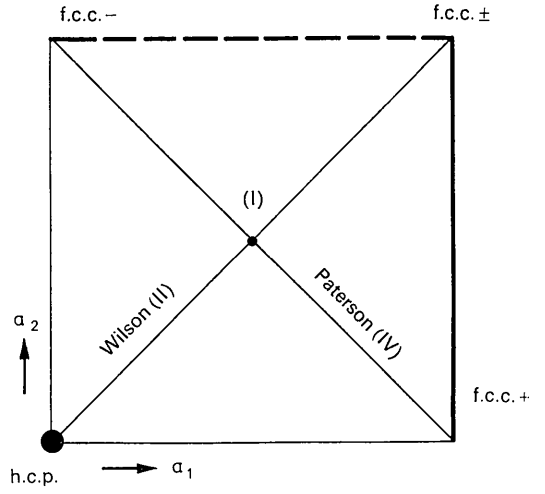

Fig. 2. The $s=2$ square for (V).

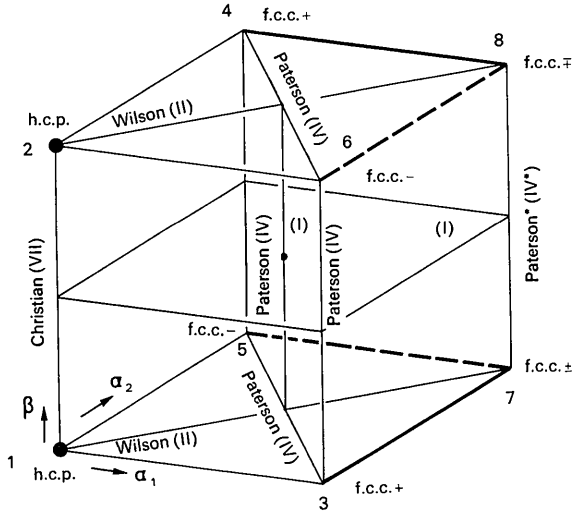

Fig. 3. The probability-cube for the new theory (V+VII).

The probability-squares (Figs. 1 and 2) for the above two theories are quite different from each other. Since the Gevers theory is concerned only with the growth and deformation faults, the Gevers square (Fig. 1) does not include the proper Paterson case (IV), although it includes the Paterson* case (IV*). On the other hand, the $s=2$ square (Fig. 2) does not include the Christian case (VII), since there the deformation fault in h.c.p. is not taken into account; the $s=2$ case (V) is no more than an extension of the Wilson case (II), where the growth fault is generalized to the extended growth fault.

Therefore, the two theories are both insufficient for interpreting experimental results on the close-packed crystals in which extended growth faults ($s\leq 2$) [necessarily including growth faults ($s\leq 2$)] and deformation faults (single) are present independently. It is desirable to propose a more general theory which includes both these theories as special cases.

A more general theory

The probability space for the new theory (V+VII) can be made up by combining α_1, α_2, and β as in Fig. 3. It is readily understood that the plane 1278 in the resulting cube corresponds to the Gevers square, and the bottom 1357 or the top 2468 to the $s=2$ square. The structures at the corners and in the edges are as indicated. The structure in the plane $\beta=0{\cdot}5$ and in the line $\alpha_1=\alpha_2=0{\cdot}5$ is the most random one (I). The Wilson case (II), the Christian case (VII), the Paterson case (IV), and the Paterson* case (IV*) are incorporated in the cube as indicated. It is to be noted that any path in the face 3768 from the edge 37 to the edge 68 corresponds to the Paterson case (IV), unless the path touches the edge 78. The same holds for the face 4857.

The nature of an *A*, *B*, or *C* layer can be characterized by the suffixes 1 and 2, which imply that the normal (not faulted) sequence to the subsequent layer is positive or negative, respectively. Then the probabilities for occurrences of all kinds of layers can be tabulated as follows.

	A_1 A_2	B_1 B_2	C_1 C_2
A_1		d_2 a_2	b_2 c_2
A_2		c_1 b_1	a_1 d_1
B_1	b_2 c_2		d_2 a_2 ,
B_2	a_1 d_1		c_1 b_1
C_1	d_2 a_2	b_2 c_2	
C_2	c_1 b_1	a_1 d_1	

(1)

where

$$\left.\begin{array}{ll} a_1=(1-\alpha_1)(1-\beta) & a_2=(1-\alpha_2)(1-\beta) \\ b_1=\alpha_1(1-\beta) & b_2=\alpha_2(1-\beta) \\ c_1=(1-\alpha_1)\beta & c_2=(1-\alpha_2)\beta \\ d_1=\alpha_1\beta & d_2=\alpha_2\beta \end{array}\right\}, \quad (2)$$

and the values at the blanks are all 0. This Table itself is the matrix **P** from which the mathematics along the lines of Kakinoki (1965, 1967) and Kakinoki & Komura (1965) starts. In the following only necessary expressions will be given.

If the fraction of the layers whose symbols have the suffix 1 (or 2) is denoted by w_1 (or w_2), we obtain

$$\left.\begin{array}{l} w_1=(1-\alpha_1)/(2-\alpha_1-\alpha_2) \\ w_2=(1-\alpha_2)/(2-\alpha_1-\alpha_2) \end{array}\right\}. \quad (3)$$

If the fraction of two-layer positive (or negative) sequences, w_+ (or w_-), is classified as above with respect to the nature of the final layer, we obtain

$$\left.\begin{array}{l} w_{+1}=w_1d_2+w_2c_1=(1-\alpha_1)\beta/(2-\alpha_1-\alpha_2) \\ w_{+2}=w_1a_2+w_2b_1=(1-\alpha_2)(1-\beta)/(2-\alpha_1-\alpha_2) \\ w_{-1}=w_1b_2+w_2a_1=(1-\alpha_1)(1-\beta)/(2-\alpha_1-\alpha_2) \\ w_{-2}=w_1c_2+w_2d_1=(1-\alpha_2)\beta/(2-\alpha_1-\alpha_2) \end{array}\right\}. \quad (4)$$

Here it is to be noted that

$$\left.\begin{array}{l} w_{+2}+w_{-1}=1-\beta \\ w_{+1}+w_{-2}=\beta \end{array}\right\}. \quad (5)$$

The fractions of the total two-layer positive and negative sequences are

$$\left.\begin{array}{l} W_+=w_{+1}+w_{+2}=[1-\alpha_2-(\alpha_1-\alpha_2)\beta]/(2-\alpha_1-\alpha_2) \\ W_-=w_{-1}+w_{-2}=[1-\alpha_1+(\alpha_1-\alpha_2)\beta]/(2-\alpha_1-\alpha_2) \end{array}\right\}, \quad (6)$$

respectively.

If the three-layer sequences as in h.c.p., $-+$ and $+-$, and those as in f.c.c., $++$ and $--$, are denoted by $h+$, $h-$, $c+$, and $c-$, respectively, their fractions are given by

$$\left.\begin{array}{l} w_{h+}=w_{-1}(a_2+d_2)+w_{-2}(b_1+c_1) \\ \quad =[(1-\alpha_1)(1-\alpha_2)-(2-3\alpha_1-3\alpha_2 \\ \quad +4\alpha_1\alpha_2)\beta(1-\beta)]/(2-\alpha_1-\alpha_2) \\ w_{h-}=w_{+1}(b_2+c_2)+w_{+2}(a_1+d_1) \\ \quad =w_{h+} \\ w_{c+}=w_{+1}(a_2+d_2)+w_{+1}(b_1+c_1) \\ \quad =W_+-w_{h+} \\ w_{c-}=w_{-1}(b_2+c_2)+w_{-2}(a_1+d_1) \\ \quad =W_--w_{h-} \end{array}\right\}. \quad (7)$$

Then the hexagonality, W_h (Sato, Itoh & Yamashita, 1964; Sato, 1966*b*; Brafman & Steinberger, 1966; Brafman, Alexander & Steinberger, 1967), and the cubicity, W_c, become

$$\left.\begin{array}{l} W_h=w_{h+}+w_{h-}=2w_{h+} \\ W_c=w_{c+}+w_{c-}=1-2w_{h+} \end{array}\right\}. \quad (8)$$

Since the unit layer has a sixfold symmetry, it is convenient to employ the unit-layer hexagonal indices $hk\,.\,\zeta$, which are related to the cubic indices HKL and the ordinary hexagonal indices $hk\,.\,l$ as

$$\left.\begin{array}{ll} h= & -H/2+K/2 \\ k= & -K/2+L/2 \\ \zeta= & H/3+K/3+L/3 \\ \zeta= & l/2 \end{array}\right\}. \quad (9)$$

As is well known, diffraction effects due to stacking faults appear only in the ζ direction, and moreover only along the reciprocal lines $h-k=\pm 1$ mod 3. It is only sufficient, therefore, to deal with diffraction intensity distributions along these lines as functions of a continuous-valued ζ.

The unitary intensity I as a function of

$$\varphi=2\pi\zeta \quad (10)$$

can be expressed to a good approximation by

$$I(\varphi)=ND(\varphi)\,, \quad (11)$$

where N is the number of unit-layers, and $D(\varphi)$ the diffuse term (Kakinoki & Komura, 1954*b*; Kakinoki, 1961, 1965, 1967):

$$D(\varphi)=1+\{\sum_1^\infty T_m \exp(-im\varphi)+\text{conj}\}\,. \quad (12)$$

Here

$$T_m=\langle V_nV^*_{n\pm m}\rangle_n/(V_0V_0^*)\,, \quad (13)$$

where the numerator is the average value of the products of the structure factors, V's, of two unit-layers separated by m interlayer spaces, and V_0 is the common unit-layer structure factor. It is to be noted that $T_0=1$ invariably. Starting from (1) we obtain

$$\begin{aligned} T_1&=\varepsilon W_+ +\varepsilon^* W_- \\ &=-\tfrac{1}{2}\pm i\frac{\sqrt{3}}{2}\,\frac{\delta'(1-2\beta)}{2-\delta}\,, \end{aligned} \quad (14)$$

where

$$\varepsilon=\exp\{2\pi i(h-k)/3\} \quad (15)$$

$$\left.\begin{array}{l} \delta=\alpha_1+\alpha_2 \\ \delta'=\alpha_1-\alpha_2 \end{array}\right\}, \quad (16)$$

and $\pm$ correspond to $h-k=\pm 1$ mod 3, respectively.

The characteristic equation for the present problem is

$$\begin{aligned} F(x)&=x^2-\{\varepsilon(\alpha_1-\delta'\beta)+\varepsilon^*(\alpha_2+\delta'\beta)\}x \\ &\qquad -(1-\delta)(1-3\gamma) \\ &=x^2+\tfrac{1}{2}\{\delta\mp i\sqrt{3}\delta'(1-2\beta)\}x \\ &\qquad -(1-\delta)(1-3\gamma)=0\,, \end{aligned} \quad (17)$$

where

$$\gamma=\beta(1-\beta)\,. \tag{18}$$

The relationship between T_m and the two solutions of (17), x_1 and x_2, is

$$T_m=c_1x_1^m+c_2x_2^m\,, \tag{19}$$

where c_1 and c_2 are two constants, which can be determined by the relations $T_0=1$ and (14).

According to Kakinoki (1965, 1967) and Kakinoki & Komura (1965), however, $D(\varphi)$ can be obtained without solving (17) and without determining c_1 and c_2. The results corresponding to $h-k=\pm1$ mod 3 are

$$\left.\begin{aligned}
&D_\pm(\varphi)=P_\pm(\varphi)/Q_\pm(\varphi)\\
&P_\pm(\varphi)=1+\alpha_1\alpha_2-(1-\delta)^2(1-3\gamma)^2+\delta'^2(1-3\gamma)\\
&\quad+\{2\alpha_1\alpha_2-\delta-\delta'^2(1-6\gamma)\}/(2-\delta)\\
&\quad-3(1-\delta)\gamma\cos\varphi\\
&\quad\mp3\sqrt{3}(1-\delta)\delta'(1-2\beta)\gamma\sin\varphi/(2-\delta)\\
&Q_\pm(\varphi)=1+\alpha_1\alpha_2+(1-\delta)^2(1-3\gamma)^2+\delta'^2(1-3\gamma)\\
&\quad+\delta\{\delta(1-3\gamma)+3\gamma\}\cos\varphi\\
&\quad-2(1-\delta)\,(1-3\gamma)\cos2\varphi\\
&\quad\mp\sqrt{3}\{2-\delta-3(1-\delta)\gamma\}\delta'(1-2\beta)\sin\varphi
\end{aligned}\right\} \tag{20}$$

$$D_\pm(\varphi)=D_\mp(-\varphi)\,. \tag{21}$$

Special choices of α_1, α_2, and β show that (20) covers the results for the Gevers case (II+VII), the $s=2$ case (V), the Wilson case (II), the Christian case (VII), the Paterson case (IV), the Paterson* case (IV*), and the most random case (I).

For powder samples, the form

$$\begin{aligned}D_p(\varphi)&=\tfrac{1}{2}\{D_+(\varphi)+D_-(\varphi)\}\\&=\tfrac{1}{2}\{D_+(\varphi)+D_+(-\varphi)\}=\tfrac{1}{2}\{D_-(\varphi)+D_-(-\varphi)\}\end{aligned} \tag{22}$$

should be used. It is to be noted, however, that

$$D_p(\varphi)=D_+(\varphi)=D_-(\varphi)=D_+(-\varphi)=D_-(-\varphi) \tag{23}$$

for the Gevers case (II+VII), and also for (II), (VII), (IV*), and (I), since all these cases are concerned with crystals with $W_-=0{\cdot}5$. The unitary intensity for powder, I_p, necessarily becomes

$$I_p(\varphi)=ND_p(\varphi)\,. \tag{24}$$

In powder diffraction experiments any deviation in φ (rad), $\Delta\varphi$ (rad), is observed as a deviation in twice the Bragg angle, $\Delta(2\theta)$. The conversion is carried out by

$$\Delta(2\theta)\,(^\circ)=\frac{180}{\pi^2}\,\frac{\cos^2\Phi}{\zeta}\,\tan\theta\,.\,\Delta\varphi\,, \tag{25}$$

where Φ is the angle between the ζ direction and the line connecting the reciprocal lattice point with the origin.

Although the general solution of the present problem has been given by (20), (22), and (24), the cases of nearly h.c.p. and nearly f.c.c. structures are most interesting. In Fig. 3 the former is represented by the vicinities of the corners 1 and 2, which are essentially equivalent to each other. Equation (22) implies that the vicinities of the edges 37, 48, 57, and 68, which represent the latter are all equivalent to each other for powders. It is only necessary, therefore, to obtain $D_p(\varphi)$ near the corner 1 and near the edge 37 and to examine them in detail.

Nearly h.c.p. structures

Since near the corner 1 of Fig. 3 α_1, α_2, and β are all small, the terms higher than second in order will be neglected. Then from (6), (8), and (14) we obtain

$$W_-=\tfrac{1}{2}-\frac{\delta'}{4} \tag{26}$$

$$W_h=1-\frac{\delta}{2}-2\beta \tag{27}$$

$$T_1=-\tfrac{1}{2}\pm i\frac{\sqrt{3}}{4}\delta'\,. \tag{28}$$

The characteristic equation (17) becomes

$$F(x)=x^2+\tfrac{1}{2}(\delta\mp i\sqrt{3}\delta')x-1+\delta+3\beta=0\,. \tag{29}$$

In the foregoing section the result was reached without obtaining x_1, x_2, c_1, and c_2 in (19). In order to make the result more comprehensible, however, it is desirable to write them explicitly. They become

$$\left.\begin{aligned}x_1&=X_1\exp(\pm i\sigma)\\x_2&=X_2\exp\{\pm i(\pi-\sigma)\}\end{aligned}\right\} \tag{30}$$

$$\left.\begin{aligned}X_1&=1-\tfrac{3}{4}\delta-\tfrac{3}{2}\beta\\X_2&=1-\tfrac{1}{4}\delta-\tfrac{3}{2}\beta\end{aligned}\right\} \tag{31}$$

$$\sigma=\frac{\sqrt{3}}{4}\delta'\,, \tag{32}$$

$$\left.\begin{aligned}c_1&=\tfrac{1}{4}(1-\tfrac{3}{2}\beta)\\c_2&=\tfrac{3}{4}(1+\tfrac{1}{2}\beta)\end{aligned}\right\} \tag{33}$$

for $h-k=\pm1$ mod 3. The summation of (12) leads to $D_\pm(\varphi)$, and (22) leads to

$$\begin{aligned}D_p(\varphi)=&\frac{c_1}{2}C(X_1,\varphi-\sigma)+\frac{c_1}{2}C(X_1,\varphi+\sigma)\\&+\frac{c_2}{2}C(X_2,\varphi-\pi-\sigma)+\frac{c_2}{2}C(X_2,\varphi-\pi+\sigma)\,,\end{aligned} \tag{34}$$

where the function C is defined as

$$C(R,\psi)=1+2\sum_1^\infty R^m\cos m\psi=\frac{1-R^2}{1+R^2-2R\cos\psi}\,. \tag{35}$$*

For $\alpha_1=\alpha_2$, (34) becomes the formula obtained by Warren (1959) for nearly h.c.p. powders of the Gevers case (II+VII).

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* The summation in (35) [or in (51) below] converges only for $|R|<1$. Note that $0<R<1$ [$R\lesssim1$ except for Y_2 of (45) below] for the present problem.

Equation (34) consists of four terms, each representing a symmetric bell-shaped curve, which has the maximum when the argument of the cosine is 0 mod 2π. Equation (10) and the last equation of (9) imply that the first two terms correspond to the reflexions with even l, and the last two to those with odd l, each slightly displaced and broadened by the presence of stacking faults. The combined function of the first two terms and that of the last two are both invariably symmetric with respect to the regular positions of reflexions. Examination of the second derivative of the first combined function at $\varphi=0$ mod 2π shows that, if the approximations (31) and (32) are employed, the first two terms invariably coalesce to give a single maximum there. Similar examination of the second combined function, on the other hand, shows that the last two terms coalesce to give a single maximum at $\varphi=\pi$ mod 2π only when:

$$\left.\begin{array}{l}\text{for } \alpha_1>\alpha_2\text{: } \alpha_1\leq 2\alpha_2+3\beta \\ \text{for } \alpha_1<\alpha_2\text{: } \alpha_2\leq 2\alpha_1+3\beta\end{array}\right\}; \qquad (36)$$

otherwise, they coalesce to give two maxima separated slightly from each other.

The integral breadth B of the reflexions with even l is readily obtained:

$$B_{\text{even}}(\text{rad})=2\pi\left\{\tfrac{3}{8}(\delta+2\beta)+\tfrac{1}{8}\frac{\delta'^2}{\delta+2\beta}\right\}, \qquad (37)$$

and B of the reflexions with odd l in the case where (36) is satisfied is

$$B_{\text{odd}}(\text{rad})=2\pi\left\{\tfrac{1}{8}(\delta+6\beta)+\tfrac{3}{8}\frac{\delta'^2}{\delta+6\beta}\right\}. \qquad (38)$$

The second terms of (37) and (38), in which the deviations from the Gevers–Warren case is reflected, are of the first order, although they each contain a small second order quantity. They drop out for $\alpha_1=\alpha_2$, and (37) and (38) become harmonized with the half-maximum breadths calculated by Warren (1959) for nearly h.c.p. powders of the Gevers case (II+VII).

If W_h is kept constant, (27) describes a plane. Variations of B_{even}, B_{odd}, $B_{\text{even}}/B_{\text{odd}}$, *etc.* in a plane of this kind, where $W_h=0{\cdot}92$ is assumed, are illustrated in Figs.4 and 5. In Fig.4 $\beta=0{\cdot}02$ is assumed, although $0\leq\beta\leq 0{\cdot}04$ for $W_h=0{\cdot}92$. The broken curves for B_{odd} near both sides show the formal numerical calculation of (38) corresponding to the doublet peak case. Fig. 5, where $\alpha_1=\alpha_2$ is assumed, corresponds to the Gevers–Warren theory for nearly h.c.p. structures.

Nearly f.c.c. structures

The mathematical treatments for the vicinity of the edge 37 of Fig.3 should be carried out in two parts. The first excludes the vicinity of the corner 7, which is the subject of the second. If we define

$$\left.\begin{array}{l}\omega_1=1-\alpha_1 \\ \omega_2=1-\alpha_2\end{array}\right\}, \qquad (39)$$

it turns out that, for the first part, ω_1 and β are small, whereas α_2 is arbitrary (but $1-\alpha_2=\omega_2$ not small), and that, for the second, ω_1, ω_2, and β are all small.

For the vicinity of the edge 37 excluding the vicinity of the corner 7, we obtain

$$W_-=\frac{\omega_1}{1-\alpha_2}+\beta \qquad (40)$$

$$W_c=1-2\omega_1-2\beta \qquad (41)$$

$$T_1=-\tfrac{1}{2}\pm i\frac{\sqrt{3}}{2}\left(1-\frac{2\omega_1}{1-\alpha_2}-2\beta\right) \qquad (42)$$

$$F(x)=x^2+\tfrac{1}{2}[1+\alpha_2-\omega_1\mp i\sqrt{3}\{(1-\alpha_2)(1-2\beta)-\omega_1\}]x +\alpha_2(1-3\beta)-\omega_1=0 \qquad (43)$$

$$\left.\begin{array}{l}x_1=Y_1\exp(\pm i\theta) \\ x_2=Y_2\exp(\mp i\theta)\end{array}\right\} \qquad (44)$$

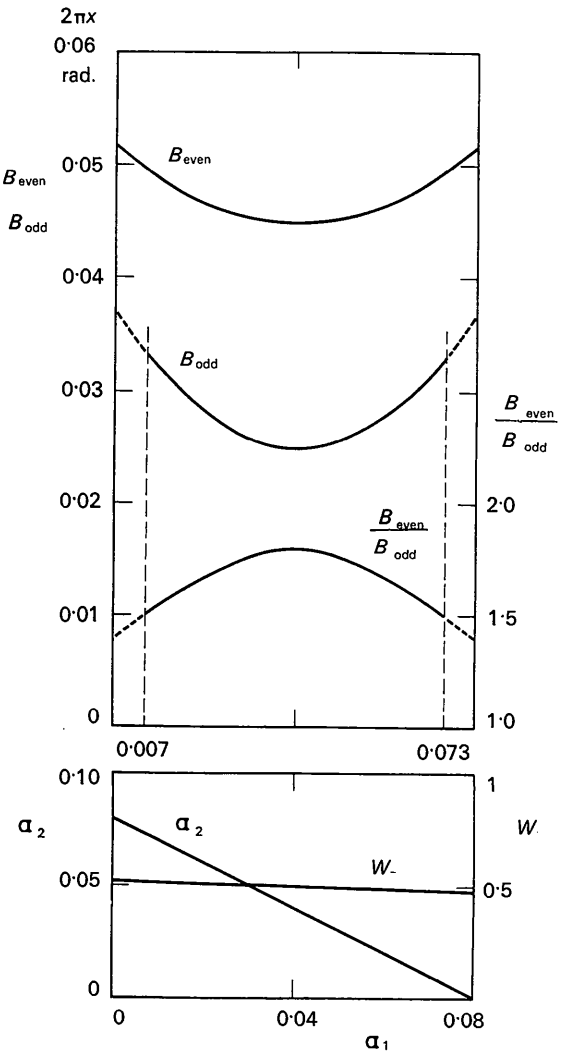

Fig.4. α_2, W_-, B_{even}, B_{odd}, and $B_{\text{even}}/B_{\text{odd}}$ *vs.* α_1, for $W_h=0{\cdot}92$ and $\beta=0{\cdot}02$.

$$\left.\begin{aligned} Y_1 &= 1-\tfrac{3}{2}\frac{1+\alpha_2}{A}\omega_1-\tfrac{3}{2}\beta \\ Y_2 &= \alpha_2\left\{1-\frac{(1-\alpha_2)(2+\alpha_2)}{2\alpha_2 A}\omega_1-\tfrac{3}{2}\beta\right\} \end{aligned}\right\} \quad (45)$$

$$\theta = \frac{2\pi}{3}+\frac{\sqrt{3}}{2}\left(\frac{1-\alpha_2}{A}\omega_1+\beta\right) \quad (46)$$

$$A = 1+\alpha_2+\alpha_2^2 \quad (47)$$

$$\left.\begin{aligned} c_1 &= (1-U)\pm iV \\ c_2 &= U\mp iV \end{aligned}\right\} \quad (48)$$

$$\left.\begin{aligned} U &= \frac{3\alpha_2(1+4\alpha_2+\alpha_2^2)}{2(1-\alpha_2)A^2}\omega_1 \\ V &= \frac{3\sqrt{3}\alpha_2(1+\alpha_2)}{2A^2}\omega_1 \end{aligned}\right\} \quad (49)$$

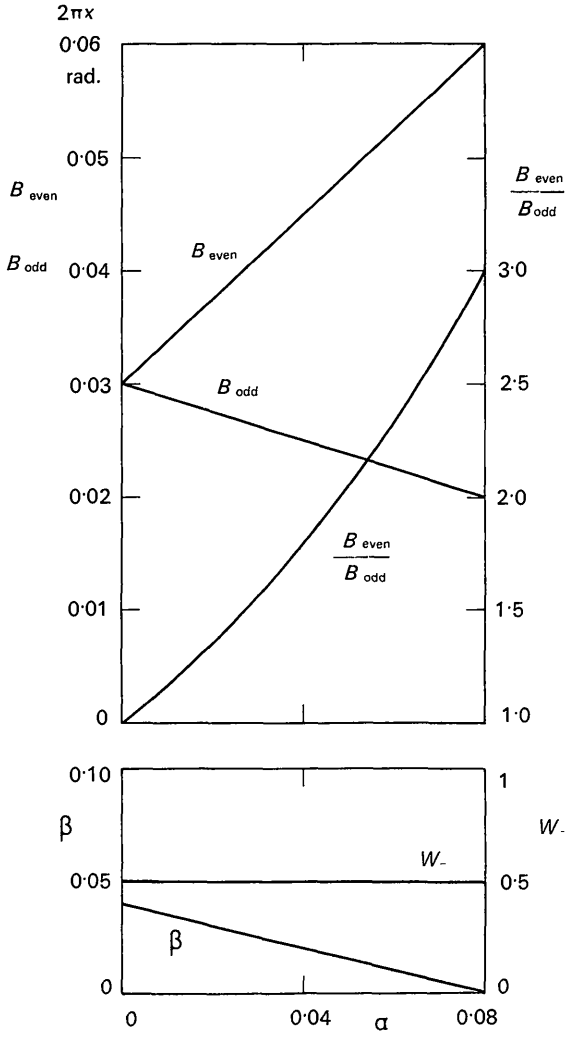

Fig. 5. β, W_-, B_{even}, B_{odd}, and $B_{\text{even}}/B_{\text{odd}}$ *vs.* α, for $W_h=0{\cdot}92$ and $\alpha_1=\alpha_2=\alpha$.

$$\begin{aligned} D_p(\varphi) = {} & \frac{1-U}{2}C(Y_1,\varphi-\theta)+\frac{V}{2}S(Y_1,\varphi-\theta) \\ & +\frac{U}{2}C(Y_2,\varphi-\theta)+\frac{V}{2}S(Y_2,\varphi-\theta) \\ & +\frac{1-U}{2}C(Y_1,\varphi+\theta)-\frac{V}{2}S(Y_1,\varphi+\theta) \\ & +\frac{U}{2}C(Y_2,\varphi+\theta)-\frac{V}{2}S(Y_2,\varphi+\theta), \end{aligned} \quad (50)$$

where, in addition to the function C of (35), the function S is defined as

$$S(R,\psi)=2\sum_1^\infty R^m \sin m\psi = \frac{2R\sin\psi}{1+R^2-2R\cos\psi}. \quad (51)$$

If, in addition to ω_1 and β, α_2 is also small, *i.e.* for the vicinity of the corner 3, (50) reduces to

$$D_p(\varphi)=\tfrac{1}{2}C(Y,\varphi-\Theta)+\tfrac{1}{2}C(Y,\varphi+\Theta), \quad (52)$$

where

$$Y=1-\tfrac{3}{2}(\omega_1+\beta) \quad (53)$$

$$\Theta=\frac{2\pi}{3}+\frac{\sqrt{3}}{2}(\omega_1+\beta). \quad (54)$$

Equation (52), which does not depend on α_2, is exactly the formula for the Paterson* case (IV*) for nearly f.c.c. structures, if $\omega_1+\beta$ is regarded as the fault probability. This situation is in harmony with the relation of the Paterson case (IV) to the corner 3 (see Fig. 3).

In the first half of (50), the first and the third terms are symmetric with respect to their maximum position, $\varphi=\theta \bmod 2\pi$, whereas the second and the fourth are asymmetric, and moreover antisymmetric, with respect to $\varphi=\theta \bmod 2\pi$. These four terms coalesce to give a reflexion close to the regular position, $\varphi=2\pi(\frac{1}{3} \bmod 1)$. Since the two antisymmetric terms are proved to affect only negligibly the maximum position of the two symmetric terms, the maximum of the combined reflexion remains at $\varphi=\theta \bmod 2\pi$. The integral breadth B of the combined reflexion consists of two parts; one is $(B/2)-b$ for the left of the maximum, and the other $(B/2)+b$ for the right of it. Almost the same applies to the other combined reflexion close to the other regular position, $\varphi=2\pi(-\frac{1}{3} \bmod 1)$, resulting from the second half of (50). Then the displacement d of the maximum from the regular position, the integral breadth B, and the asymmetry b/B are calculated to be

$$d\,(\text{rad})=\pm\frac{\sqrt{3}}{2}\left(\frac{1-\alpha_2}{A}\omega_1+\beta\right) \quad (55)$$

$$B\,(\text{rad})=2\pi\left\{(1-U)\frac{1+Y_1}{1-Y_1}+U\frac{1+Y_2}{1-Y_2}\right\}^{-1} \quad (56)$$

$$\frac{b}{B}=\pm\frac{V}{\pi}\ln\left(\frac{1+Y_1}{1-Y_1}\,\frac{1+Y_2}{1-Y_2}\right), \quad (57)$$

where $\pm$ correspond to the reflexions whose regular positions are at $\varphi=2\pi(\pm\frac{1}{3} \bmod 1)$, respectively.

On the other hand, for the vicinity of the corner 7, we obtain

$$W_-=(\omega_1-\Delta'\beta)/\Delta \tag{58}$$

$$W_c=1-2\omega_1\omega_2/\Delta-2\beta \tag{59}$$

$$\left.\begin{aligned}\Delta&=\omega_1+\omega_2\\ \Delta'&=\omega_1-\omega_2\end{aligned}\right\} \tag{60}$$

$$T_1=-\tfrac{1}{2}\mp i\,\frac{\sqrt{3}}{2}\,\frac{\Delta'(1-2\beta)}{\Delta} \tag{61}$$

$$F(x)=x^2+\tfrac{1}{2}(2-\Delta\pm i\sqrt{3}\Delta')x+1-\Delta-3\beta=0 \tag{62}$$

$$\left.\begin{aligned}x_1&=Z_1\exp(\pm i\tau)\\ x_2&=Z_2\exp(\mp i\tau)\end{aligned}\right\} \tag{63}$$

$$\left.\begin{aligned}Z_1&=1-\omega_1-\tfrac{3}{2}\beta\\ Z_2&=1-\omega_2-\tfrac{3}{2}\beta\end{aligned}\right\} \tag{64}$$

$$\tau=\frac{2\pi}{3}+\frac{\sqrt{3}}{2}\beta \tag{65}$$

$$\left.\begin{aligned}c_1&=\omega_2/\Delta\pm i\omega_1\omega_2/(\sqrt{3}\Delta)\\ c_2&=\omega_1/\Delta\mp i\omega_1\omega_2/(\sqrt{3}\Delta)\end{aligned}\right\} \tag{66}$$

$$\begin{aligned}D_p(\varphi)=&\frac{\omega_2}{2\Delta}C(Z_1,\varphi-\tau)+\frac{\omega_1\omega_2}{2\sqrt{3}\Delta}S(Z_1,\varphi-\tau)\\ &+\frac{\omega_1}{2\Delta}C(Z_2,\varphi-\tau)+\frac{\omega_1\omega_2}{2\sqrt{3}\Delta}S(Z_2,\varphi-\tau)\\ &+\frac{\omega_2}{2\Delta}C(Z_1,\varphi+\tau)-\frac{\omega_1\omega_2}{2\sqrt{3}\Delta}S(Z_1,\varphi+\tau)\\ &+\frac{\omega_1}{2\Delta}C(Z_2,\varphi+\tau)-\frac{\omega_1\omega_2}{2\sqrt{3}\Delta}S(Z_2,\varphi+\tau)\,.\end{aligned} \tag{67}$$

For $\omega_1=\omega_2$, eight terms of (67) reduce to four, two symmetric and two antisymmetric, and (67) becomes the formula obtained by Warren (1959) for nearly f.c.c. powders of the Gevers case (II+VII).

An examination of (67), similar to that of (50), leads to the following:

$$d\,(\text{rad})=\pm\frac{\sqrt{3}}{2}\beta \tag{68}$$

$$B\,(\text{rad})=2\pi\left(\frac{\omega_2}{\Delta}\frac{1+Z_1}{1-Z_1}+\frac{\omega_1}{\Delta}\frac{1+Z_2}{1-Z_2}\right)^{-1} \tag{69}$$

$$\frac{b}{B}=\pm\frac{\omega_1\omega_2}{\sqrt{3}\pi\Delta}\ln\left(\frac{1+Z_1}{1-Z_1}\frac{1+Z_2}{1-Z_2}\right), \tag{70}$$

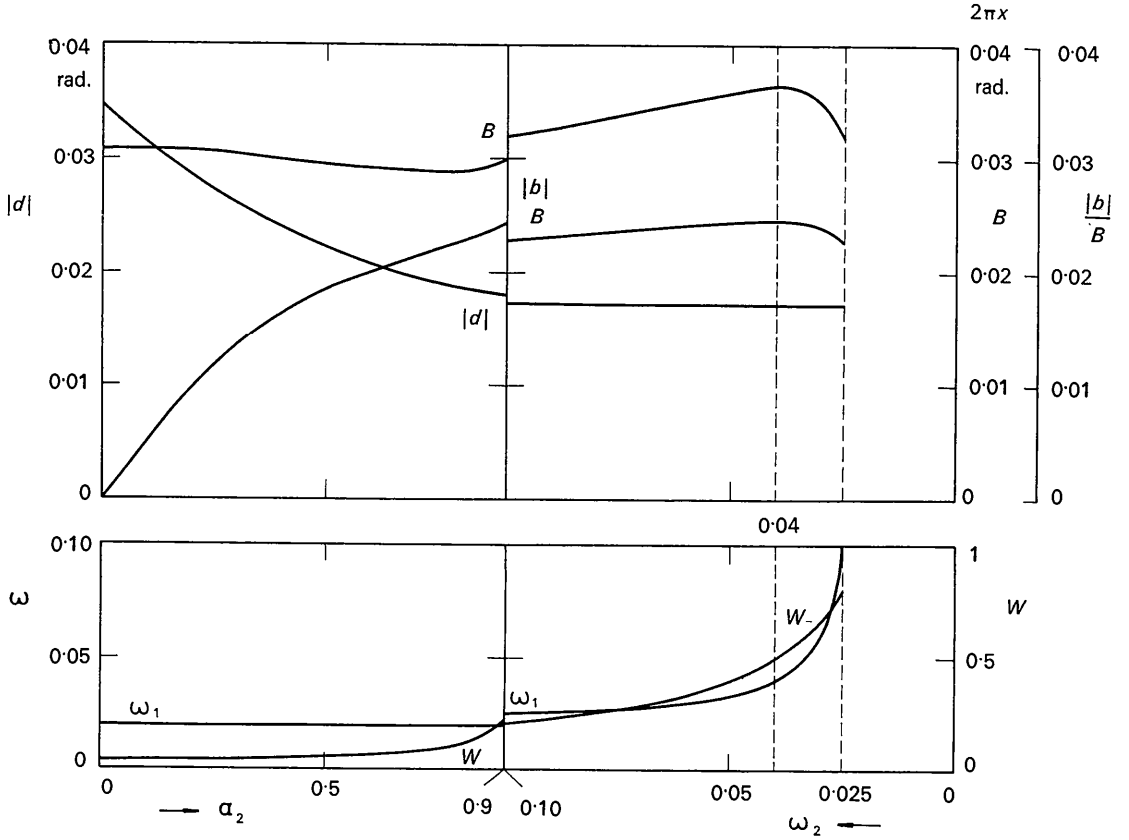

Fig. 6. ω_1, W_-, $|d|$, B, and $|b|/B$ *vs.* α_2(or ω_2), for $W_c=0{\cdot}92$ and $\beta=0{\cdot}02$. For $\alpha_2\leq 0{\cdot}9$, (40), (41), (55), (56), and (57) are used, and for $\omega_2\leq 0{\cdot}10$, (58), (59), (68), (69), and (70) are used.

where ± correspond, as before, to the reflexions whose regular positions are at $\varphi = 2\pi(\pm\frac{1}{3} \bmod 1)$, respectively.

Now, if W_c is kept constant, (41) and (59) describe a plane and a curved surface, respectively. Variations of $|d|$, B, $|b|/B$, *etc.* in a plane or a curved surface of this kind, where $W_c = 0{\cdot}92$ is assumed, are illustrated in Figs. 6 and 7. In Fig. 6 $\beta = 0{\cdot}02$ is assumed, although $0 \leq \beta \leq 0{\cdot}04$ for $W_c = 0{\cdot}92$. The misfits in Fig. 6 at $\alpha_2 = 0{\cdot}9$ ($\omega_2 = 0{\cdot}10$) are ascribed to the approximations employed. It is to be noted that B and $|b|/B$ become a maximum at $\omega_1 = \omega_2 = 0{\cdot}04$, where $W_- = 0{\cdot}5$ (the Gevers–Warren case). Fig. 7, where $\omega_1 = \omega_2$ is assumed, corresponds to the Gevers–Warren theory for nearly f.c.c. structures.

Discussion

In the foregoing sections, the diffuse terms $D_p(\varphi)$ [see (12), (22), and (24)] for nearly h.c.p. and nearly f.c.c. structures have been written in the form corresponding to that reached after the summation of the series (12) has been achieved. This form allows the explicit expression of peak displacement, broadening, and asymmetry. Peak displacements and integral breadths in degrees of the Debye–Scherrer rings are calculated from (25), if d's of (55) and (68) and B's of (37), (38), (56), and (69) are regarded as $\Delta\varphi$ (rad) in (25). Asymmetries are given by (57) and(70).

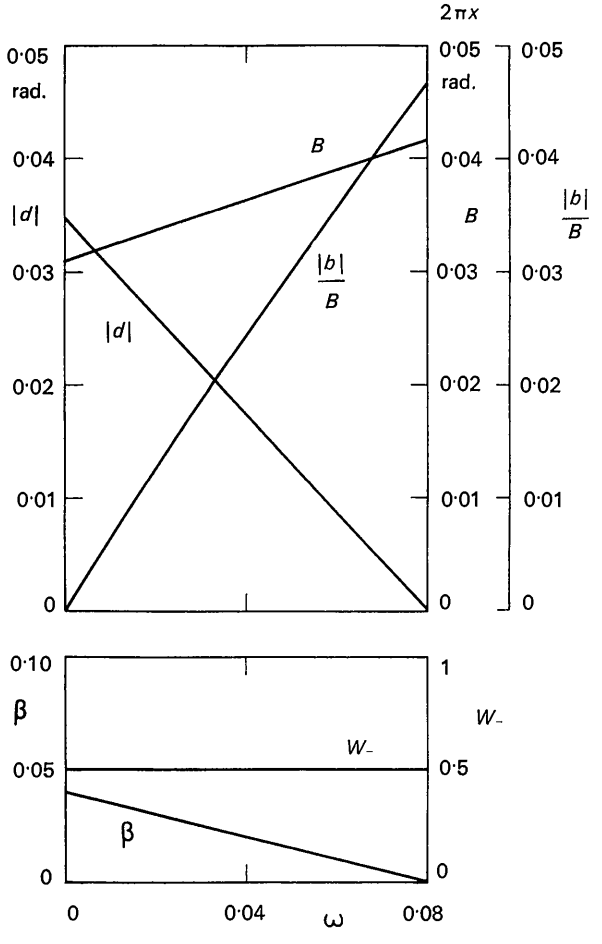

Fig. 7. β, W_-, $|d|$, B, and $|b|/B$ *vs.* ω, for $W_c = 0{\cdot}92$ and $\omega_1 = \omega_2 = \omega$.

Fairly stable statistical structures intermediate between two standard stacking patterns seem to be generally described by $s \geq 3$. Two examples of such a case are CdS, intermediate between the hexagonal and the cubic modifications (Sato, 1962), and Cu_3Al β' martensite between 2- and 18-layer standard structures (Nishiyama, Kakinoki & Kajiwara, 1965; Kajiwara, 1967). In these examples 'fault' probabilities, which can take quite large values, should be understood, regardless of their literal implication, as parameters describing statistical modes of layer stacking (Kakinoki, 1966*a*). Nevertheless, for metal and alloy powders prepared, *e.g.* by filing, 'fault' probabilities seems to be a good terminology, since they describe mistakes in a standard stacking, taking invariably small values. In this case, it may be justifiable to employ the lowest possible s, *i.e.* $s = 2$, at least to the first approximation. It has been found, on the other hand, that the deformation faults actually observed in metals and alloys are almost only of the *single* (*intrinsic* for f.c.c.) type (Hashimoto, Howie & Whelan, 1962; Howie & Valdrè, 1963; Art, Gevers & Amelinckx, 1963). Thus we believe that the present general theory, based on the extended growth fault with $s = 2$ (V) [necessarily including (IV), (II), and (I)] and the *single* deformation fault in h.c.p. (VII), is suitable for the interpretion of experimental results on metal and alloy powders.

In principle, the three fault probabilities, $\alpha_1(\omega_1)$, $\alpha_2(\omega_2)$, and β, of a nearly h.c.p. or f.c.c. powder sample can be determined, if the experimental results are dealt with according to the present theory. Such exact determinations may, however, be extremely difficult, because of practical limitations in the quality of the diffraction experiments.

The information obtained from the diffraction experiments on nearly h.c.p. powders is generally poor, since neither peak displacement nor asymmetry are found. Moreover, in Fig. 4 for $\alpha_1 \neq \alpha_2$, the variation of the ratio of the integral breadths, $B_{\text{even}}/B_{\text{odd}}$, is not remarkable. Thus the Gevers–Warren theory for $\alpha_1 = \alpha_2$ emerges as a practical, though rough, approximation to the present theory. Once this theory is assumed, the two fault probabilities, $\alpha(=\alpha_1=\alpha_2)$ and β, can be determined by use of Fig. 5, where the variation of $B_{\text{even}}/B_{\text{odd}}$ is considerable.

For a nearly f.c.c. powder, generally peak displacement and asymmetry occur, in addition to broadening. Fig. 6 implies that, among these three quantities, the asymmetry $|b|/B$ varies most remarkably, and that, if $|b|/B$ is considerable, the point representing the structure in the probability-cube (Fig. 3) is near the corner 7. In the right-hand half of Fig. 6 for $\omega_1 \neq \omega_2$, however, none of the variations of $|d|$, B, and $|b|/B$ are remark-

able. Thus the Gevers–Warren theory for $\omega_1=\omega_2$ emerges again as a practical, though rough, approximation. Once this theory is assumed, the two fault probabilities, $\omega(=\omega_1=\omega_2)$ and β, can be determined by use of Fig. 7. On the other hand, if the asymmetry is very slight, the point is near either the corner 3 (see the left hand half of Fig. 6) or the edge 78 (see Fig. 7). The stacking faults in this case are mainly of the Paterson type, and it is in principle impossible to determine whether the point is near the corner 3 or near the edge 78, so far as the powder diffraction is concerned.

The Gevers–Warren theory is being widely employed for interpreting stacking faults in powders of metals, alloys, and other materials of h.c.p. and f.c.c. (and, additionally, b.c.c. and other) structures. Reviews on such lines have been given by Warren (1959), Wagner (1966), and Mikkola & Cohen (1966). Strain and particle-size effects discussed in these reviews are beyond the scope of the present paper. It must be emphasized, however, that the Gevers–Warren theory is no more than a very simplified case of the more general theory proposed in the present paper. Therefore, the growth fault probability α or ω and the deformation fault probability β deduced from the Gevers–Warren theory should be taken as very rough approximations. This situation should be particularly emphasized for the former, α or ω, since $\alpha=\alpha_1=\alpha_2$ or $\omega=\omega_1=\omega_2$, which leads necessarily to $W_-=0{\cdot}5$, is generally not the case for particles of actual powder samples. Roughly speaking, the growth fault probability deduced from this theory should be taken as the average of two extended growth fault probabilities, $(\alpha_1+\alpha_2)/2$ or $(\omega_1+\omega_2)/2$. Nevertheless, so far as powder diffraction is concerned, we are obliged to be content with this theory in view of the poor quality of diffraction experiments. Finally, it is noted again that the terms 'growth' and 'deformation' should be used carefully; as has been mentioned in the last paragraph of the introduction, they characterize only the geometry of stacking sequences.

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