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# X-ray Diffraction from Close-Packed Structures with Stacking Faults. II. *hhc* Crystals

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The kinematical theory of X-ray diffraction by *hhc* (samarium-type) crystals with growth and deformation faults is developed. The intensity distribution in reciprocal space is derived as a function of five parameters which represent three growth and two deformation fault probabilities. Only reflexions with $H-K\neq 3N$, $N$ an integer, are affected by faulting and exhibit generally changes in integrated intensity, profile peak shift, broadening and asymmetry. It is shown that nine independent combinations of the five fault probabilities can be evaluated from the measured profile characteristics.

## Introduction

Extensive work has been performed on the derivation of X-ray diffraction effects of faulting in close-packed structures with ranges of influence equal to 2 and 3 (Warren, 1959; Anantharaman, Rama Rao & Lele, 1972). The diffraction effects of growth and deformation faults in *hcc* crystals were described in an earlier paper (Lele, 1974) while those in *hhc* crystals are considered here. Both of these structures have a range of influence equal to 4. Gevers (1954) has given a general treatment for growth faults in crystals of this type. We shall extend this work by including deformation faults in our treatment as also by relating the fault probabilities directly to the experimentally observable diffraction effects.

The *hhc* structure, exhibited for example by samarium, can be considered as a layer structure produced by the regular stacking of close-packed layers in the sequence *ABCBCACAB,A* where the letters *A*, *B* and *C* denote the three possible positions of the close-packed layers and the comma marks the completion of the repeat period. The geometrical structure factors for different *H*, *K*, *L* are given in Table 1. The possible growth and deformation faults along with a different notation due to Nabarro (1967), virtual processes for their formation and stacking sequences containing the faults (indicated by vertical bar) are given in Table 2. The following calculations have been made under assumptions usual in this type of work (see, *e.g.*, Prasad & Lele, 1971).

Table 2. *Stacking faults in hhc crystals*

| Fault | Notation | Process of formation | Stacking sequence |
|---|---|---|---|
| Growth | *c* | Insertion of 1 layer + glide | *c h h c*   *c h h c*<br>*B A B C* \| *A C A B* |
| | *h* | Twin | *h c h h*   *h c h h*<br>*B C B C* \| *B A B A* |
| | *hc* | Twin | *h h c h*   *c h h c*<br>*A B C B* \| *A B A C* |
| Deformation | *hhc* | Glide | *h h c h*   *c h h h*<br>*A B C B* \| *A B A B* |
| | 3*c* | Glide | *c h h c*   *c c c h*<br>*B A B C* \| *A B C B* |

## Diffraction from faulted crystals

Following Warren (1959), the diffracted intensity is given by

$$I(h_3)=\psi^2\sum_m\langle\exp(i\Phi_m)\rangle\exp(2\pi imh_3/9) \qquad (1)$$

where

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

$q_m$ being a stochastic variate equal to 0, 1 or 2 respectively according as the $m$ layer is *A*, *B* or *C* when the origin layer is *A*. Values of $q_m$ for *B* and *C* layers at the origin can be obtained by cyclic permutation. Further

$$\langle\exp(i\Phi_m)\rangle=C\varrho^m \qquad (3)$$

Table 1. *Structure factors for hhc crystals*

| $H-K$ \ $L$ | $9M$ | $\|F\|$ $9M\mp1$ | $9M\pm2$ | $9M\mp4$ |
|---|---|---|---|---|
| $3N$ | $9f$ | 0 | 0 | 0 |
| $3N\pm1$ | 0 | $3f\left(1+2\cos\frac{4\pi}{9}\right)$ | $3f\left(1+2\cos\frac{8\pi}{9}\right)$ | $3f\left(1+2\cos\frac{2\pi}{9}\right)$ |

Note: $F=0$ for $H-K+L\neq 3N$

where $\varrho$ is a solution of the so-called characteristic equation and $C$ can be obtained from the initial conditions. The characteristic equation for growth faults has been obtained by Gevers [1954, equation (12)] while that for deformation faults is derived in an Appendix. Combining these two equations, we have finally

$$\varrho^6+\alpha_c\varrho^5+(1-\alpha_c-\alpha_h-\alpha_{hc}-3\alpha_{3c})\varrho^3+2\alpha_c\varrho^2 +(1-2\alpha_c-2\alpha_h-2\alpha_{hc}-6\alpha_{hhc}-3\alpha_{3c})=0 \quad \text{for } \alpha\text{'s} \ll 1 \quad (4)$$

where $\alpha_x$ is the probability of the occurrence of faults of type $x$ (Table 2). For convenience, the relationship to Gevers' (1954) notation is given below

$$\alpha_c \to \alpha_3=\alpha_4;\quad \alpha_h \to (1-\alpha_1);\quad \alpha_{hc} \to \alpha_2 .$$

Solutions of equation (4) may be expressed in the following form

$$\varrho_\nu=Z_\nu \exp(-2\pi i)\left(\frac{\nu}{9}+X_\nu\right) \quad \nu=1,2,4,5,7 \;\&\; 8 \quad (5)$$

where $Z_\nu$ and $X_\nu$ are real and are given by

$$Z_\nu=1-\frac{\alpha_c}{3}\left(1-\cos\frac{4\pi\nu}{9}\right)-\frac{\alpha_h}{3}-\frac{\alpha_{hc}}{3}-\alpha_{hhc}-\frac{\alpha_{3c}}{2}$$
$$X_\nu=\frac{\alpha_c}{6\pi}\sin\frac{4\pi\nu}{9}+\frac{\alpha_{hhc}}{3\pi}\sin\frac{2\pi\nu}{3}-\frac{\alpha_{3c}}{6\pi}\sin\frac{2\pi\nu}{3}$$
$$\nu=1,2,4,5,7 \;\&\; 8 . \quad (6)$$

The initial conditions, required for evaluation of the $C_\nu$'s and found by direct evaluation from all possible stacking sequences of six layers, are given below

$$\left.\begin{aligned}
&\langle\exp(i\Phi_0)\rangle=1\\
&\langle\exp(i\Phi_1)\rangle=-\tfrac{1}{2}\\
&\langle\exp(i\Phi_2)\rangle=(\tfrac{1}{2})\left(1-\frac{2\alpha_c}{3}-\frac{\alpha_h}{3}-\frac{\alpha_{hc}}{3}-2\alpha_{3c}\right)\\
&\langle\exp(i\Phi_3)\rangle=-(\tfrac{1}{2})(1-\alpha_c-3\alpha_{3c})\\
&\langle\exp(i\Phi_4)\rangle=(\tfrac{1}{3})(-2\alpha_c+\alpha_h+2\alpha_{hc}+6\alpha_{hhc}-3\alpha_{3c})\\
&\langle\exp(i\Phi_5)\rangle=(\tfrac{1}{6})(5\alpha_c-4\alpha_h-2\alpha_{hc}-12\alpha_{hhc}+9\alpha_{3c})
\end{aligned}\right] \quad (7) .$$

Substituting from equations (5), (6) and (7) in equation (3) and solving the resultant set of six simultaneous equations for the $C_\nu$'s, we have

$$\begin{aligned}
C_1&=0{\cdot}1008\,\{1+0{\cdot}4089\,(\alpha_h-\alpha_{hc})-0{\cdot}2176\alpha_{hhc} -1{\cdot}1573\alpha_{3c}-i[0{\cdot}09\,(\alpha_h+\alpha_{hc})-1{\cdot}3514\alpha_{hhc} +1{\cdot}4067\alpha_{3c}]\}\\
C_2&=0{\cdot}043\,\{1-1{\cdot}4705\,(\alpha_h-\alpha_{hc})-0{\cdot}9598\alpha_{hhc} -0{\cdot}1938\alpha_{3c}+i[0{\cdot}318\,(\alpha_h+\alpha_{hc})-2{\cdot}182\alpha_{hhc} +1{\cdot}4794\alpha_{3c}]\}\\
C_4&=0{\cdot}3562\,\{1+0{\cdot}0616\,(\alpha_h-\alpha_{hc})+0{\cdot}1774\alpha_{hhc} +0{\cdot}351\alpha_{3c}-i[0{\cdot}7466\,(\alpha_h+\alpha_{hc})+0{\cdot}6457\alpha_{hhc} -0{\cdot}5767\alpha_{3c}]\} . \quad (8)\\
C_5&=C_4^*\\
C_7&=C_2^*\\
C_8&=C_1^*
\end{aligned}$$

where the * denotes complex conjugation. Substituting from equations (3) and (5) in (1), we have on simplification

$$\begin{aligned}
I(h_3)=\psi^2 &\Big[C_{1r}\sum_m Z_1^{|m|}\cos 2\pi m\left(\frac{h_3}{9}-\tfrac{1}{9}-X_1\right) -C_{1i}\sum_m Z_1^{|m|}\sin 2\pi\,|m|\left(\frac{h_3}{9}-\tfrac{1}{9}-X_1\right)\Big]\\
+\psi^2 &\Big[C_{2r}\sum_m Z_2^{|m|}\cos 2\pi m\left(\frac{h_3}{9}-\tfrac{2}{9}-X_2\right) -C_{2i}\sum_m Z_2^{|m|}\sin 2\pi|m|\left(\frac{h_3}{9}-\tfrac{2}{9}-X_2\right)\Big]\\
+\psi^2 &\Big[C_{4r}\sum_m Z_4^{|m|}\cos 2\pi m\left(\frac{h_3}{9}-\tfrac{4}{9}-X_4\right) -C_{4i}\sum_m Z_4^{|m|}\sin 2\pi|m|\left(\frac{h_3}{9}-\tfrac{4}{9}-X_4\right)\Big]\\
+\psi^2 &\Big[C_{4r}\sum_m Z_4^{|m|}\cos 2\pi m\left(\frac{h_3}{9}-\tfrac{5}{9}+X_4\right) +C_{4i}\sum_m Z_4^{|m|}\sin 2\pi\,|m|\left(\frac{h_3}{9}-\tfrac{5}{9}+X_4\right)\Big]\\
+\psi^2 &\Big[C_{2r}\sum_m Z_2^{|m|}\cos 2\pi m\left(\frac{h_3}{9}-\tfrac{7}{9}+X_2\right) +C_{2i}\sum_m Z_2^{|m|}\sin 2\pi|m|\left(\frac{h_3}{9}-\tfrac{7}{9}+X_2\right)\Big]\\
+\psi^2 &\Big[C_{1r}\sum_m Z_1^{|m|}\cos 2\pi m\left(\frac{h_3}{9}-\tfrac{8}{9}+X_1\right) +C_{1i}\sum_m Z_1^{|m|}\sin 2\pi|m|\left(\frac{h_3}{9}-\tfrac{8}{9}+X_1\right)\Big] \quad (9)
\end{aligned}$$

where $C_{\nu r}$ and $C_{\nu i}$ are the real and imaginary parts of $C_\nu$ and are given by

$$C_{\nu r}=(\tfrac{1}{2})(C_\nu+C_\nu^*);\quad C_{\nu i}=(\tfrac{1}{2i})(C_\nu-C_\nu^*) \quad \nu=1,2,4 . \quad (10)$$

Performing the summations in equation (9), we have

$$\begin{aligned}
I(h_3)=\;&\psi^2C_{1r}\,\frac{1-Z_1^2-2(C_{1i}/C_{1r})\,Z_1\sin 2\pi\left(\frac{h_3}{9}-\frac{1}{9}-X_1\right)}{1+Z_1^2-2Z_1\cos 2\pi\left(\frac{h_3}{9}-\frac{1}{9}-X_1\right)}\\
+\;&\psi^2C_{2r}\,\frac{1-Z_2^2-2(C_{2i}/C_{2r})\,Z_2\sin 2\pi\left(\frac{h_3}{9}-\frac{2}{9}-X_2\right)}{1+Z_2^2-2Z_2\cos 2\pi\left(\frac{h_3}{9}-\frac{2}{9}-X_2\right)}\\
+\;&\psi^2C_{4r}\,\frac{1-Z_4^2-2(C_{4i}/C_{4r})\,Z_4\sin 2\pi\left(\frac{h_3}{9}-\frac{4}{9}-X_4\right)}{1+Z_4^2-2Z_4\cos 2\pi\left(\frac{h_3}{9}-\frac{4}{9}-X_4\right)}
\end{aligned}$$

$$+\psi^2 C_{4r} \frac{1-Z_4^2+2(C_{4i}/C_{4r})\,Z_4 \sin 2\pi\left(\frac{h_3}{9}-\frac{5}{9}+X_4\right)}{1+Z_4^2-2Z_4\cos 2\pi\left(\frac{h_3}{9}-\frac{5}{9}+X_4\right)}$$

$$+\psi^2 C_{2r} \frac{1-Z_2^2+2(C_{2i}/C_{2r})\,Z_2 \sin 2\pi\left(\frac{h_3}{9}-\frac{7}{9}+X_2\right)}{1+Z_2^2-2Z_2\cos 2\pi\left(\frac{h_3}{9}-\frac{7}{9}+X_2\right)}$$

$$+\psi^2 C_{1r} \frac{1-Z_1^2+2(C_{1i}/C_{1r})\,Z_1 \sin 2\pi\left(\frac{h_3}{9}-\frac{8}{9}+X_1\right)}{1+Z_1^2-2Z_1\cos 2\pi\left(\frac{h_3}{9}-\frac{8}{9}+X_1\right)}\,. \qquad (11)$$

### Description of diffraction effects

Reflexions with $H-K=3N$, $L=9M$, $M$ and $N$ integers, remain sharp. For reflexions with $H-K\neq 3N$, the first to sixth terms on the right-hand side of equation (11) give rise to broadened peaks corresponding to $L=9M+1$, $9M+2$, $9M+4$, $9M+5$, $9M+7$, $9M+8$ respectively. In general, all reflexions exhibit changes in integrated intensity, profile peak shift, profile broadening and profile asymmetry. These effects can be utilized for estimating fault probabilities. Quantitative expressions for these profile characteristics are given below.

*Profile integrated intensity*

The integrated intensities $T_1$, $T_2$ and $T_4$ in reciprocal space for reflexions with $L=9M\pm 1, 9M\pm 2$ and $9M\pm 4$ respectively can be obtained by integrating separately the corresponding terms on the right-hand side of equation (11) with respect to $h_3$. The fractional changes in the ratios $R_{21}$ and $R_{41}$ of the integrated intensities $T_2$, $T_1$ and $T_4$, $T_1$ respectively are given by

$$\Delta R_{21}/R_{21} = -1{\cdot}8794\,(\alpha_h-\alpha_{hc}) - 0{\cdot}7422\,\alpha_{hhc} + 0{\cdot}9635\,\alpha_{3c} \qquad (12)$$

$$\Delta R_{41}/R_{41} = -0{\cdot}3473\,(\alpha_h-\alpha_{hc}) + 0{\cdot}3950\,\alpha_{hhc} + 1{\cdot}5083\,\alpha_{3c}\,. \qquad (13)$$

By experimental measurement of the quantities $\Delta R_{21}/R_{21}$ and $\Delta R_{41}/R_{41}$, one obtains two different combinations of the fault probabilities. We designate such a combination by the term compound fault parameter.

*Profile peak shift*

Each term on the right-hand side of equation (11) gives rise to a peak when the argument of the cosine term in the denominator is a multiple of $2\pi$. The changes in the profile peak positions due to faulting can thus be found and after conversion to $2\theta°$ coordinates are given by

$$\Delta(2\theta_m)_1^0 = \pm\frac{270\sqrt{3}}{\pi^2}\cdot\frac{|L|d^2}{c^2} \times \tan\theta\,(1{\cdot}1372\,\alpha_c+2\alpha_{hhc}-\alpha_{3c}) \quad \text{for } L=9M\pm 1 \qquad (14)$$

$$\Delta(2\theta_m)_2^0 = \pm\frac{270\sqrt{3}}{\pi^2}\cdot\frac{|L|d^2}{c^2} \times \tan\theta\,(0{\cdot}3949\,\alpha_c-2\alpha_{hhc}+\alpha_{3c}) \quad \text{for } L=9M\pm 2 \qquad (15)$$

$$\Delta(2\theta_m)_4^0 = \pm\frac{270\sqrt{3}}{\pi^2}\cdot\frac{|L|d^2}{c^2} \times \tan\theta\,(-0{\cdot}7422\,\alpha_c+2\alpha_{hhc}-\alpha_{3c}) \quad \text{for } L=9M\pm 4\,. \qquad (16)$$

Profile peak shift measurements thus lead to estimates of three more compound fault parameters. However, only two of these are independent.

*Profile integral breadth*

The integral breadth is defined as the ratio of the profile integrated intensity and the profile maximum. Considering each of the terms in equation (11) separately and converting to $2\theta°$ coordinates, we have

$$(\beta_f)_1^0 = \frac{270}{\pi}\cdot\frac{|L|d^2}{c^2} \times \tan\theta\,(1{\cdot}6527\,\alpha_c+2\alpha_h+2\alpha_{hc}+6\alpha_{hhc}+3\alpha_{3c}) \quad \text{for } L=9M\pm 1 \qquad (17)$$

$$(\beta_f)_2^0 = \frac{270}{\pi}\cdot\frac{|L|d^2}{c^2} \times \tan\theta\,(3{\cdot}8794\,\alpha_c+2\alpha_h+2\alpha_{hc}+6\alpha_{hhc}+3\alpha_{3c}) \quad \text{for } L=9M\pm 2 \qquad (18)$$

$$(\beta_f)_4^0 = \frac{270}{\pi}\cdot\frac{|L|d^2}{c^2} \times \tan\theta\,(0{\cdot}4679\,\alpha_c+2\alpha_h+2\alpha_{hc}+6\alpha_{hhc}+3\alpha_{3c}) \quad \text{for } L=9M\pm 4\,. \qquad (19)$$

Three additional compound fault parameters can, therefore, be obtained from measurements of $(\beta_f)_1^0$, $(\beta_f)_2^0$ and $(\beta_f)_4^0$. Again, however, only two of these are independent.

*Profile asymmetry*

A simple measure of profile asymmetry is the shift of the centroid of a profile from its peak position. Following Cohen & Wagner (1962), we have from equation (9)

$$\Delta(2\theta_{c-m})_1^0 = \pm \frac{360 \ln 2}{\pi^2} \times \tan\theta\,[0{\cdot}09\,(\alpha_h+\alpha_{hc}) - 1{\cdot}3514\,\alpha_{hhc} + 1{\cdot}4067\,\alpha_{3c}] \quad \text{for } L=9M\pm1 \quad (20)$$

$$\Delta(2\theta_{c-m})_2^0 = \pm \frac{360 \ln 2}{\pi^2} \times \tan\theta\,[-0{\cdot}318\,(\alpha_h+\alpha_{hc}) + 2{\cdot}182\,\alpha_{hhc} - 1{\cdot}4794\,\alpha_{3c}] \quad \text{for } L=9M\pm2 \quad (21)$$

$$\Delta(2\theta_{c-m})_4^0 = \pm \frac{360 \ln 2}{\pi^2} \times \tan\theta\,[0{\cdot}7466\,(\alpha_h+\alpha_{hc}) + 0{\cdot}6457\,\alpha_{hhc} - 0{\cdot}5767\,\alpha_{3c}] \quad \text{for } L=9M\pm4\,. \quad (22)$$

Thus, measurement of asymmetry leads to estimates of three more compound fault parameters.

## Discussion

Independent estimates of a total of nine compound fault parameters can be obtained from measurements of the profile characteristics mentioned above. Since there are only five fault probabilities, we have an over-determined set of equations and all five fault probabilities can be found in principle. In practice, all the data required may not be available with sufficient accuracy and further the profile broadening may include effects due to small domains and strains within the specimen. Methods for eliminating the latter effects are considered, for example, by Anantharaman, Rama Rao & Lele (1972). Analysis in any given situation would depend on the data available and the probable effects present in the sample and as such will not be considered here.

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## APPENDIX

### Characteristic equation for deformation faults

We consider three types of layers to be present in the perfect *hhc* structure according as they continue the stacking in a *ch*, *hh* or *c* way. We further note that *hhc* faults can occur only after the first two types of layers while 3*c* faults can occur only after *c*-type layers (Table 2). The transition probabilities as also the phase differences from the $(m-1)$ to the $m$ layer for the above three types are shown in Table 3. Let $\Phi_m^y$ represent the phase difference for an $m$ layer of the type $y$ where $y$ is one of *ch*, *hh* and *c*.

Table 3. *Probability trees giving transition probabilities and phase differences from one layer to the next*

| $(m-1)$ layer | Probability | $m$ layer | Phase difference |
|---|---|---|---|
| *hh* A | $1-\alpha_{hhc}$ | *c* B | $+\varphi_0$ |
| | $\alpha_{hhc}$ | *c* C | $-\varphi_0$ |
| *ch* A | $1-\alpha_{hhc}$ | *hh* B | $+\varphi_0$ |
| | $\alpha_{hhc}$ | *hh* C | $-\varphi_0$ |
| *c* A | $1-\alpha_{3c}$ | *ch* C | $-\varphi_0$ |
| | $\alpha_{3c}$ | *ch* B | $+\varphi_0$ |

Then from Table 3, we have

$$\langle\exp(i\Phi_m^c)\rangle = \{(1-\alpha_{hhc})\omega + \alpha_{hhc}\omega^*\}\,\langle\exp(i\Phi_{m-1}^{hh})\rangle \quad \text{(A1)}$$

$$\langle\exp(i\Phi_m^{hh})\rangle = \{(1-\alpha_{hhc})\omega + \alpha_{hhc}\omega^*\}\,\langle\exp(i\Phi_{m-1}^{ch})\rangle \quad \text{(A2)}$$

$$\langle\exp(i\Phi_m^{ch})\rangle = \{(1-\alpha_{3c})\omega^* + \alpha_{3c}\omega\}\,\langle\exp(i\Phi_{m-1}^{c})\rangle \quad \text{(A3)}$$

where

$$\omega = \exp(2\pi i/3)(H-K) = \exp(i\varphi_0)\,. \quad \text{(A4)}$$

Replacing $m$ by $(m-1)$ and $(m-2)$ respectively in equations (A2) and (A3) and eliminating $\langle\exp(i\Phi_{m-1}^{hh})\rangle$ and $\langle\exp(i\Phi_{m-2}^{ch})\rangle$ from the resulting equations and equation (A1), we obtain

$$\langle\exp(i\Phi_m^c)\rangle = \{(1-\alpha_{hhc})\omega + \alpha_{hhc}\omega^*\}^2 \times \{(1-\alpha_{3c})\omega^* + \alpha_{3c}\omega\}\,\langle\exp(i\Phi_{m-3}^{c})\rangle\,. \quad \text{(A5)}$$

Let the solution of this recurrence equation be of the form

$$\langle\exp(i\Phi_m^c)\rangle = C\varrho^m\,. \quad \text{(A6)}$$

Substituting from equation (A6) in (A5), we get

$$\varrho^3 - \{(1-\alpha_{hhc})\omega + \alpha_{hhc}\omega^*\}^2 \times \{1-\alpha_{3c})\omega^* + \alpha_{3c}\omega\} = 0\,. \quad \text{(A7)}$$

It can be shown that, for crystals in the twin orientation, the complex conjugate of the above equation holds. Thus

$$\varrho^3 - \{(1-\alpha_{hhc})\omega^* + \alpha_{hhc}\omega\}^2 \times \{(1-\alpha_{3c})\omega + \alpha_{3c}\omega^*\} = 0\,. \quad \text{(A8)}$$

The same relations can be shown to hold for *ch* and *hh* layers also. For a crystal simultaneously containing *h* or *hc* faults (which arise from twinning operations, Table 2), some parts of the crystal are in the normal orientation and others in the twin orientation. A general equation covering this situation is obtained by multiplying equations (A7) and (A8) giving on simplification

$$\varrho^6+(1-3\alpha_{3c})\varrho^3+(1-6\alpha_{hhc}-3\alpha_{3c})=0 \quad \text{for } \alpha\text{'s} \ll 1 \qquad \text{(A9)}$$

where terms with squares and higher powers of the fault probabilities as also their cross products have been omitted.


**References**

ANANTHARAMAN, T. R., RAMA RAO, P. & LELE, S. (1972.) *Recent Developments in Metallurgical Science and Technology*, pp. 407–484. New Delhi: Indian Institute of Metals.

COHEN, J. B. & WAGNER, C. N. J. (1962). *J. Appl. Phys.* **33**, 2073–2077.

GEVERS, R. (1954). *Acta Cryst.* **7**, 337–343.

LELE, S. (1974). *Acta Cryst.* **A30**, 509–513.

NABARRO, F. R. N. (1967). *Theory of Crystal Dislocations.* Oxford Univ. Press.

PRASAD, B. & LELE, S. (1971). *Acta Cryst.* **A27**, 54–64.

WARREN, B. E. (1959). *Progr. Metal Phys.* **8**, 147–202.


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# X-ray Diffraction from Close-Packed Structures with Stacking Faults. III. *hhcc* Crystals

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The kinematical theory of X-ray diffraction by *hhcc* crystals with stacking faults is developed. The intensity distribution in reciprocal space is derived as a function of seven parameters which represent four growth and three deformation fault probabilities. Only reflexions with $H-K\neq 3N$, $N$ an integer, are affected by faulting and exhibit generally changes in integrated intensity, profile peak shift, broadening and asymmetry. It is shown that eleven independent combinations of the seven fault probabilities can be evaluated from the measured profile characteristics.

## Introduction

Extensive work has been performed on the derivation of X-ray diffraction effects of faulting in close-packed structures with ranges of influence equal to 2 and 3 (Warren, 1959; Anantharaman, Rama Rao & Lele, 1972). Three structures with a range of influence equal to 4 are possible. Diffraction effects of growth and deformation faults for two of these, namely *hcc* and *hhc* structures, have been treated in earlier papers (Lele, 1974*a,b*) while Gevers (1954) has given a general treatment for growth faults in crystals of this type. In the present paper we shall consider the third structure, namely *hhcc*, containing growth and deformation faults.

The 12-layered *hhcc* structure can be considered as a layer structure produced by the regular stacking of close-packed layers in the sequence *ABACBCBACACB*, *A* where the letters *A*, *B* and *C* denote the three possible positions of the close-packed layers and the comma marks the completion of the repeat period. The geometrical structure factors for different *H*, *K*, *L* are given in Table 1. The possible growth and deformation faults along with a different notation due to Nabarro (1967), virtual processes for their formation and stacking sequences containing the faults (indicated by vertical bar) are given in Table 2. The following calculations have been made under assumptions usual in this type of work (see, *e.g.*, Prasad & Lele, 1971).

## Diffraction from faulted crystals

Following Warren (1959), the diffracted intensity is given by

$$I(h_3)=\psi^2\sum_m\langle\exp(i\Phi_m)\rangle\exp(2\pi imh_3/12) \qquad (1)$$

where

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

$q_m$ being a stochastic variate equal to 0, 1 or 2 respectively according as the $m$ layer is $A$, $B$ or $C$ when the origin layer is $A$. Cyclic permutation yields the values of $q_m$ for $B$ and $C$ layers at the origin. Further,

$$\langle\exp(i\Phi_m)\rangle=C\varrho^m \qquad (3)$$

where $\varrho$ is a solution of the so-called characteristic equation and $C$ can be obtained from the initial conditions. The characteristic equation for growth faults has been obtained by Gevers (1954, equation 12) while that for deformation faults is derived in the Appendix. Combining these two equations, we have finally

$$\varrho^8+\alpha_c\varrho^7+\alpha_{hhc}\varrho^5+(1-\alpha_h-\alpha_c-\alpha_{hhc}-\alpha_{cch}-3\alpha_{4h}-6\alpha_{2hc})\varrho^4-\alpha_c\varrho^3-\alpha_{hhc}\varrho+(1-2\alpha_h-2\alpha_c-2\alpha_{hhc}-2\alpha_{cch}-3\alpha_{4h}-6\alpha_{2hc}-3\alpha_{4c})=0 \quad \text{for } \alpha\text{'s}\ll 1 \qquad (4)$$

where $\alpha_x$ is the probability of the occurrence of faults of type $x$ (Table 2). For convenience, the relationship