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Diffraction by Crystals with Planar Faults. I. General Theory

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Kinematical diffraction from a crystal having planar faults is described by a systematic writing of the Patterson function and its Fourier transform for the general case of an arbitrary number of different kinds of layer, describing the faults in terms of a fault vector plus an addition, or subtraction, of scattering matter. The general series expression is readily simplified to deal with a wide variety of special cases. Particular examples include Wadsley-type shear faults associated with non-stoichiometry of oxides and the deformation and growth faults of simple close-packed structures.

1. Introduction

The problem of calculating diffraction intensities for crystals having planar faults has been treated by many authors. The literature abounds with solutions ranging from the very elegant and general (Jagodzinski, 1949*a*,*b*,*c*; 1954, Kakinoki & Komura, 1952, 1954*a*,*b*; 1965; Kakinoki, 1967) to the relatively simple and direct treatments of particular cases (see Warren, 1969). The only possible justification for our presentation of yet another treatment is that a somewhat different formulation of the diffraction problem appears to lead by readily comprehended steps to a general solution from which it is relatively easy to derive expressions which are particularly suited to the description of diffraction from some commonly occurring types of disorder.

In recent years a great deal of evidence has been obtained by X-ray or electron diffraction and, in particular, by direct images of crystal structures in the electron microscope (Allpress & Sanders, 1973; Iijima, 1973; Cowley & Iijima, 1975) that variations of stoichiometry of inorganic materials may be accommodated by the existence of planar faults at which there is a local variation of the cation/anion ratio. Such faults may take the form of shear planes (Wadsley faults), micro-twins or more complicated configurations and may occur in disordered, partially ordered or well ordered arrays.

Streaking in diffraction patterns has frequently been observed and attributed to such faults but detailed calculations of diffraction intensities for such cases have not been made. The occurrence of a modification of the structure at the fault plane adds considerable complication to the diffraction calculations.

An approach to the diffraction problem which is particularly suited to this type of fault structure was evolved in the course of the efforts to understand the streaking observed in electron diffraction patterns of magnesium fluorogermanate which are described in part II of this series (Cowley, 1976). It was soon realized that a generalization of the same type of treatment would provide a convenient means for dealing with a much wider range of diffraction problems and indicate the basis for useful approximations which would allow rapid prediction of the type of diffraction effects to be expected. In this paper we present the general formulation for kinematical diffraction, with some examples of applications to relatively simple, familiar types of faulting.

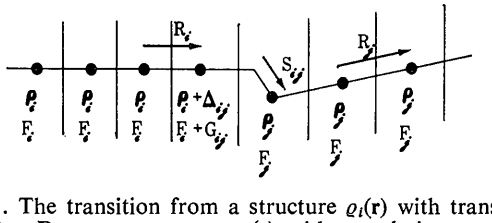

Fig. 1. The transition from a structure $\varrho_i(\mathbf{r})$ with translation vector $\mathbf{R}_i$, to a structure $\varrho_j(\mathbf{r})$ with translation vector $\mathbf{R}_j$ through a fault layer of content $\varrho_i+\Delta_{ij}$ and a shift vector $\mathbf{S}_{ij}$.

2. Most general formulation

We consider a crystal to be made up of an arbitrary number of different types of layer. For kinematical X-ray diffraction, we characterize the i type of layer by an electron-density distribution function $\varrho_i(\mathbf{r})$ referred to some suitably chosen origin. When only i-type layers are present the ordered stacking is given by a translation vector $\mathbf{R}_i$ between equivalent origin points of the layers. When a fault occurs, the sequence of layers of content $\varrho_i(\mathbf{r})$ with translation vector $\mathbf{R}_i$ changes to a sequence of layers of content $\varrho_j(\mathbf{r})$ with translation vector $\mathbf{R}_j$. No assumptions regarding the translation vectors within the layers need be made. When such a fault occurs, the ϱ_i layer at the fault is modified by the addition (or subtraction) of electron density, $\Delta_{ij}(\mathbf{r})$, and the vector $\mathbf{R}_i$ is modified to $\mathbf{R}_i+\mathbf{S}_{ij}$ (see Fig. 1).

We assume initially that the probability for such a fault is α_{ij}. The implied assumption that the faults occur at random subject to this one probability value

is not so restrictive as may first appear. If particular sequences of planes of atoms tend to recur, each of these sequences may be described as a separate type of layer. Thus, in the terminology of Jagodzinski (1949*a*), it is possible to include the effect of a *Reichweite* greater than unity.

The *a priori* probability of occurrence of an i-type layer, g_i, is given by equating transitions to and from the i type as

$$g_i=(\sum_j g_j\alpha_{ji})/\sum_j \alpha_{ij}\,. \tag{1}$$

We now write the generalized Patterson function $P(\mathbf{r})$ in terms of components involving $0,1,2,\ldots$ interlayer vectors $\mathbf{R}_n$. The zero component involving only intralayer vectors can be written

$$P_0(\mathbf{r})=N\sum_i g_i[(1-A_i)\{\varrho_i(\mathbf{r})*\varrho_i(-\mathbf{r})\} + \sum_j \alpha_{ij}(\varrho_i+\Delta_{ij})*(\varrho_i+\Delta_{ij})], \tag{2}$$

where we have put $A_i=\sum_j\alpha_{ij}$, so that $(1-A_i)$ is probability that an i layer will not be modified by a fault. The summation over j gives the intralayer vectors for layers modified by faults. The total number of layers is N.

Fourier transforming (2) gives the corresponding contribution to the intensity:

$$I_0/N=\sum_i g_i[(1-A_i)|F_i|^2+\sum_j \alpha_{ij}|F_i+G_{ij}|^2], \tag{3}$$

where F_i and G_{ij} are the Fourier transforms of ϱ_i and Δ_{ij} respectively.

For vectors between nearest-neighbor layers we write down, in turn, the components for the various possible pairs. The origin layer may be ϱ_i, followed by either ϱ_i or $\varrho_i+\Delta_{ij}$, or the origin layer may be $\varrho_i+\Delta_{ij}$ followed by either ϱ_j or $\varrho_j+\Delta_{jk}$, so that

$$\begin{aligned}P_1(\mathbf{r})=N\sum_i g_i\delta(\mathbf{r}-\mathbf{R}_i)*[\varrho_i(-\mathbf{r})*\{(1-A_i)\varrho_i(\mathbf{r}) \\ +\sum_j\alpha_{ij}(\varrho_i+\Delta_{ij})\}+\sum_j\alpha_{ij}\delta(\mathbf{r}-\mathbf{S}_{ij})*\{\varrho_i(-\mathbf{r}) \\ +\Delta_{ij}(-\mathbf{r})\}*\{(1-A_j)\varrho_j+\sum_k\alpha_{jk}(\varrho_j+\Delta_{jk})\}].\end{aligned}$$

Fourier transforming then gives

$$\begin{aligned}I_1/N&=\sum_i\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}_i\}\,[g_i(1-A_i)F_i^*\{(1-A_i)F_i \\ &\quad+\sum_j\alpha_{ij}(F_i+G_{ij})\}+g_i\sum_j\alpha_{ij}(F_i^*+G_{ij}^*) \\ &\quad\times\exp\{2\pi i\mathbf{u}\,.\,\mathbf{S}_{ij}\}\,.\,\{(1-A_j)F_j \\ &\quad+\sum_k\alpha_{jk}(F_j+G_{jk})\}] \\ &=\sum_i g_i[(1-A_i)F_i^*\{F_i+\sum_j\alpha_{ij}G_{ij}\} \\ &\quad+\sum_j\alpha_{ij}(F_i^*+G_{ij}^*)\exp\{2\pi i\mathbf{u}\,.\,\mathbf{S}_{ij}\} \\ &\quad\times\{F_j+\sum_k\alpha_{jk}G_{jk}\}]\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}\}\,.\end{aligned} \tag{4}$$

In this and subsequent terms, we have the recurring expression

$$F_i+\sum_j\alpha_{ij}G_{ij}\equiv F_i'\,, \tag{5}$$

which represents the average i-type structure amplitude.

For vectors between second-nearest layers we may write down, similarly, all possible layer pairs and Fourier transform to give, using (5),

$$\begin{aligned}I_2/N&=\sum_i g_iF_i^*\exp\{2\pi i\mathbf{u}\,.\,2\mathbf{R}_i\}\,[(1-A_i)F_i' \\ &\quad+\sum_j\alpha_{ij}F_j'\exp\{2\pi i\mathbf{u}\,.\,\mathbf{S}_{ij}\}] \\ &\quad+\sum_i g_i\sum_j\alpha_{ij}(F_i^*+G_{ij}^*) \\ &\quad\times\exp\{2\pi i\mathbf{u}\,.\,(\mathbf{R}_i+\mathbf{R}_j+\mathbf{S}_{ij})\}\,.\,[(1-A_j)F_j' \\ &\quad+\sum_k\alpha_{jk}F_k'\exp\{2\pi i\mathbf{u}\,.\,\mathbf{S}_{jk}\}]\,.\end{aligned}$$

This and subsequent terms may be written more simply if we put

$$B_i\equiv(1-A_i)F_i'+\sum_j\alpha_{ij}F_j'\exp\{2\pi i\mathbf{u}\,.\,\mathbf{S}_{ij}\}, \tag{6}$$

which may be regarded as an average structure amplitude for an i-type layer plus its possible neighbors.

Similarly we may write the contributions for third-nearest, fourth-nearest neighbor layers and so on, and see a consistent pattern emerging from which the general expression can be deduced. For vectors $-\mathbf{R}_i$ in the opposite direction we obtain the terms $I_{-n}/N=I_n^*/N$.

We may separate out contributions from sets of vectors which include no fault. These give series of the form

$$1+(1-A_i)\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}_i\} +(1-A_i)^2\exp\{2\pi i\mathbf{u}\,.\,2\mathbf{R}_i\}+\ldots$$

which are summed to give

$$[1-(1-A_i)\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}_i\}]^{-1}.$$

The expression for the total intensity is then written as a series of terms involving no faults, one fault only, two faults only and so on:

$$\begin{aligned}I/N&=\sum_i g_i(1-A_i)|F_i|^2+\sum_i g_i\sum_j\alpha_{ij}|F_i+G_{ij}|^2 \\ &\quad+\sum_i g_i(1-A_i)F_i^*\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}_i\} \\ &\quad\times\left[F_i'+\frac{\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}_i\}}{1-(1-A_i)\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}_i\}}\left[B_i\right.\right. \\ &\quad+\sum_j\alpha_{ij}\frac{\exp\{2\pi i\mathbf{u}\,.\,(\mathbf{R}_j+\mathbf{S}_{ij})\}}{1-(1-A_j)\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}_j\}}\left[B_j\right. \\ &\quad\left.\left.+\sum_k\alpha_{jk}\frac{\exp\{2\pi i\mathbf{u}\,.\,(\mathbf{R}_k+\mathbf{S}_{jk}\}}{1-(1-A_k)\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}_k\}}\left[B_k+\ldots\right]\right]\right] \\ &\quad+\sum_i g_i\sum_j\alpha_{ij}(F_i^*+G_{ij}^*)\exp\{2\pi i\mathbf{u}\,.\,(\mathbf{R}_i+\mathbf{S}_{ij})\} \\ &\quad\times\left[F_j'+\frac{\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}_j\}}{1-(1-A_j)\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}_j\}}\left[B_j\right.\right. \\ &\quad\left.\left.+\ldots\right]\right]+\text{c.c.}\,.\end{aligned} \tag{7}$$

The components corresponding to vectors starting on non-fault planes and fault planes are written separately. The initial terms in these two parts are different but the bracket starting with B_j and subsequent brackets are identical. In these expressions the addition of each bracket introduces the possibility of a further fault.

If the probability of faults is low, only a small number of brackets needs to be considered to give a good representation of the intensity distribution. There will tend to be maxima of intensity, as expected, when $\mathbf{u} \cdot \mathbf{R}_i$ is close to an integer, *i.e.* near the positions of the reciprocal-lattice points for the ordered stacking of the individual types of layer.

The expression (7) can be applied in principle to cases of much greater complication than are normally met in practice. Its chief virtue is that it may be simplified considerably, often giving series which may be summed algebraically for particular cases of interest.

3. Special cases

(1) *All* $G_{ij}=0$

In many situations, the modification of the structures of the layers at the fault planes is negligibly small. In some cases, the influence of even large modifications on the intensities of interest may be small (see part II). If in equation (7) we put all $G_{ij}=0$ there is a considerable simplification. Instead of (5) and (6) we have

$$F_i'=F_i\,,$$
$$B_i=(1-A_i)F_i+\sum_j \alpha_{ij}F_j \exp\{2\pi i\mathbf{u}\cdot\mathbf{S}_{ij}\}\,. \qquad (8)$$

The two parts of (7) may then be combined to give a single series:

$$I/N=\sum_i \frac{g_iF_i^*}{1-(1-A_i)\exp\{2\pi i\mathbf{u}\cdot\mathbf{R}_i\}}\Big[F_i + \sum_j \frac{\alpha_{ij}\exp\{2\pi i\mathbf{u}\cdot(\mathbf{R}_i+\mathbf{S}_{ij})\}}{1-(1-A_j)\exp\{2\pi i\mathbf{u}\cdot\mathbf{R}_j\}}\Big[F_j + \sum_k \frac{\alpha_{jk}\exp\{2\pi i\mathbf{u}\cdot(\mathbf{R}_j+\mathbf{S}_{jk})\}}{1-(1-A_k)\exp\{2\pi i\mathbf{u}\cdot\mathbf{R}_k\}}\Big[F_k+\ldots\Big]\Big]\Big] + \text{c.c.} - \sum_i g_i|F_i|^2. \qquad (9)$$

(2) *One type of layer only*: $G=0$

A particularly simple case is that for which there is only one type of layer, with a probability α that a fault occurs which displaces the layers by a vector $\mathbf{S}$ with no modification of the layers at the fault. Then (9) becomes

$$I/N=\frac{F^*}{1-(1-\alpha)\exp\{2\pi i\mathbf{u}\cdot\mathbf{R}\}}\Big[F + \frac{\alpha\exp\{2\pi i\mathbf{u}\cdot(\mathbf{R}+\mathbf{S})\}}{1-(1-\alpha)\exp\{2\pi i\mathbf{u}\cdot\mathbf{R}\}}\Big[F + \frac{\alpha\exp\{2\pi i\mathbf{u}\cdot(\mathbf{R}+\mathbf{S})}{1-(1-\alpha)\exp\{2\pi i\mathbf{u}\cdot\mathbf{R}\}}\Big[F+\ldots\Big]\Big]\Big] + \text{c.c.} - |F|^2.$$

The expression in square brackets is a geometric series which sums to give

$$F\Big[1-\frac{\alpha\exp\{2\pi i\mathbf{u}\cdot(\mathbf{R}+\mathbf{S})\}}{1-(1-\alpha)\exp\{2\pi i\mathbf{u}\cdot\mathbf{R}\}}\Big]^{-1},$$

so that

$$\begin{aligned} I/N&=|F|^2[\{1-(1-\alpha)\exp\{2\pi i\mathbf{u}\cdot\mathbf{R}\} \\ &\quad -\alpha\exp\{2\pi i\mathbf{u}\cdot(\mathbf{R}+\mathbf{S})\}\}^{-1}+\text{c.c.}-1] \\ &=|F|^2\alpha(1-\alpha)\,(1-\cos 2\pi\mathbf{u}\cdot\mathbf{S}) \\ &\quad\times[1-\alpha+\alpha^2-(1-\alpha)\cos 2\pi\mathbf{u}\cdot\mathbf{R} \\ &\quad -\alpha\cos 2\pi\mathbf{u}\cdot(\mathbf{R}+\mathbf{S})+\alpha(1-\alpha)\cos 2\pi\mathbf{u}\cdot\mathbf{S}]^{-1}. \end{aligned} \qquad (10)$$

If α is small, this gives peaks of intensities close to the reciprocal-lattice points for which $\mathbf{u}\cdot\mathbf{R}$ is an integer, except when $\mathbf{u}\cdot\mathbf{S}$ is nearly integral. The intensity maxima are actually displaced from these reciprocal-lattice points by an amount proportional to α. Thus if $2\pi\mathbf{u}\cdot\mathbf{R}=2\pi n+\varepsilon$, the displacement of the maximum of intensity is given by minimizing the denominator with respect to ε as

$$\varepsilon=-\alpha\sin(2\pi\mathbf{u}\cdot\mathbf{S})/\{1-\alpha(1-\cos 2\pi\mathbf{u}\cdot\mathbf{S})\}\,, \qquad (11)$$

and the maximum intensity value is

$$I_{\max}/N\simeq 2|F|^2(1+\alpha)/\alpha(1-\cos 2\pi\mathbf{u}\cdot\mathbf{S}). \qquad (12)$$

The magnitude and direction of the displacements of the intensity maxima from the reciprocal-lattice point may be seen to correspond to those given by intuitive appreciation of the way in which the fault vector $\mathbf{S}$ tends to modify the average periodicities of the structure.

A particular case of such an intensity distribution is discussed in part II. Many observations of intensity maxima displaced from reciprocal-lattice-point positions have been reported and discussed in the literature. Notable examples include the diffuse scattering associated with heavy radiation-damage effects in close-packed metals and oxides (Austerman & Miller, 1965; Keating, 1968; Nimura, 1955) and the diffuse scattering associated with the β–ω transformations of various Ti and Zr alloys (Moss, Keating & Axe, 1973; Borie, Sass & Andreassen, 1973). In each case an analysis of the scattering in terms of the model we have used here provides an immediate indication of the type of fault involved and the approximate frequency of occurrence of the fault. If, as in the latter example, the individual layers are of finite extent, the broadening of the diffuse peaks in directions parallel to the layers may often, to a good approximation, be treated separately.

(3) *One type of layer only*: $G\neq 0$

If, as in some types of Wadsley faults in non-stoichiometric oxides, there is only one type of layer but this is modified at the shear plane, the expression equivalent to (10) derived from the general solution (7) includes terms in $|F|^2$, $|G|^2$ and the real and imaginary parts of F^*G, thus:

$$I(\mathbf{u})/N=\alpha(1-\alpha)\,[|F|^2(1-\cos 2\pi\mathbf{u}\,.\,\mathbf{S})$$
$$+(\mathrm{Re}\,F^*G)\,\{1+\cos 2\pi\mathbf{u}\,.\,(\mathbf{R}+\mathbf{S})$$
$$-\cos 2\pi\mathbf{u}\,.\,\mathbf{R}-\cos 2\pi\mathbf{u}\,.\,\mathbf{S}\}$$
$$-(\mathrm{Im}\,F^*G)\,\{\sin 2\pi\mathbf{u}\,.\,\mathbf{R}+(1-2\alpha)\sin 2\pi\mathbf{u}\,.\,\mathbf{S}$$
$$-\sin 2\pi\mathbf{u}\,.\,(\mathbf{R}+\mathbf{S})\}$$
$$+|G|^2(1-\cos 2\pi\mathbf{u}\,.\,\mathbf{R})]$$
$$\times[1-\alpha+\alpha^2-(1-\alpha)\cos 2\pi\mathbf{u}\,.\,\mathbf{R}$$
$$-\alpha\cos 2\pi\mathbf{u}\,.\,(\mathbf{R}+\mathbf{S})$$
$$+\alpha(1-\alpha)\cos 2\pi\mathbf{u}\,.\,\mathbf{S}]^{-1}. \qquad (13)$$

It may seem from this expression that the faulted layers contribute an inordinately large amount to the intensity since G occurs with the same weighting as F in spite of the fact that the ratio of faulted to non-faulted layers is α. However it may be noted that for α small the intensity maxima occur very close to the reciprocal-lattice points given by $\mathbf{u}\,.\,\mathbf{R}$ integral and when $\cos 2\pi\mathbf{u}\,.\,\mathbf{R}=1$ all the terms in the first square bracket of (13) vanish except for the term in $|F|^2$. Hence if, as often happens, it is the positions and relative heights of the intensity maxima which are the main points of interest, the assumption that $G=0$ will not lead to serious errors (see part II).

4. *Non-random faults*

The tendency for faults to cluster together or to avoid one another can be introduced readily by taking sums of intensity expressions. For the simple case of one type of fault only and $G=0$, for example, if the expression (10) is denoted by $I_\alpha(u)$, we may consider an intensity distribution

$$I(\mathbf{u})=aI_\alpha(\mathbf{u})+cI_\gamma(\mathbf{u}), \qquad (14)$$

where $a+c=1$ and $a\alpha+c\gamma>0$. This will represent a situation where the probability of no fault in n layers takes the form

$$a(1-\alpha)^n+c(1-\gamma)^n. \qquad (15)$$

If $\gamma>\alpha$ and c is positive, the effect is to make the probability of a fault greater for small n than for large n. If c is negative with $\gamma>\alpha$, the effect will be to decrease the probability of a fault for small n, *i.e.* the fault planes will tend to avoid each other.

For nearest-neighbor planes, for example, the probability of a fault will be $a\alpha+c\gamma$ which is less than α for c negative, while for n large the fault probability per layer becomes $a\alpha$ which is greater than α. For the general expression (7), the introduction of non-random faulting is correspondingly more complicated.

5. *Faults in close-packed structures*

In order to demonstrate some of the virtues of this type of approach, we consider briefly its application to the familiar case of faulting in simple, close-packed structures. As is customary we describe the sequence of close-packed hexagonal layers by the notation *ABABAB*... for the h.c.p. and *ABCABCA*... for the f.c.c. structure and represent the packing sequence, with faults, by diagrams of the sections of the structures on (110) planes, as in Fig. 2. It is sufficient to consider the two-dimensional unit cells with x axes in the planes of the layers and the c axes corresponding to the interlayer $\mathbf{R}$ vectors used in our general treatment.

For h.c.p. structures we consider a c axis equal to the c axis of the normal two-layer unit cell. Growth faults give sequences *ABABCBCB*... or *ABABACAC*... Hence there are two types of fault occurring with equal probability. One fault, occurring at $z=0$ gives a shift vector $\mathbf{S}_1=(\frac{1}{3})\mathbf{A}+(\frac{1}{2})\mathbf{c}$ with one plane of atoms added. The other fault occurring at $z=\frac{1}{2}$ gives a shift $\mathbf{S}_2=-(\frac{1}{3})\mathbf{a}-(\frac{1}{2})\mathbf{c}=-\mathbf{S}_1$ and one plane of atoms is subtracted.

Deformation faults in h.c.p. structures can also be described in terms of two types of fault having equal probability. A fault at the $z=0$ level has a shift vector $\mathbf{S}=-\mathbf{a}/3$ with no modification of the structure. The other fault, at $z=\frac{1}{2}$, has a shift vector $\mathbf{S}=\mathbf{a}/3$ but at the fault the layer structure changes from the normal *AB* sequence, with one atom at (0,0) and one at $(-\frac{1}{3},\frac{1}{2})$.

For f.c.c. structures it is convenient to take an oblique unit cell with the c axis, for example, from an *A* position in one layer to a *B* or *C* position in the next. There are thus two translation vectors $\mathbf{R}_1$ and $\mathbf{R}_2$, corresponding to the two equivalent packing sequences *ABCABC*... or *ACBACB*... (see Fig. 2). A growth fault corresponds to a change from one translation vector to the other, with no change of layer structure and shift vector $\mathbf{S}=0$. A deformation fault is characterized by a shift vector $\mathbf{S}=\mathbf{a}/3$ for the stacking sequence defined by translation vector $\mathbf{R}_1$ and by $\mathbf{S}=-\mathbf{a}/3$ for the $\mathbf{R}_2$ variant.

For each of these cases the form of the diffraction

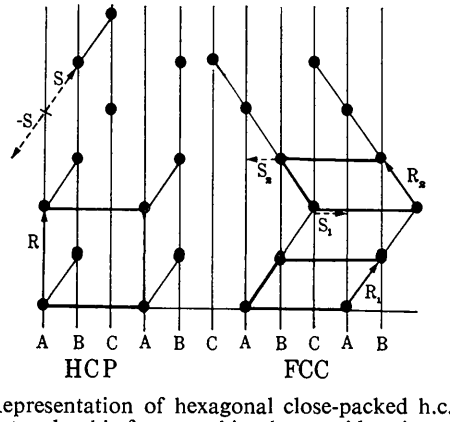

Fig. 2. Representation of hexagonal close-packed h.c.p. and face-centered cubic f.c.c. stacking by consideration of atom positions on a (110) plane. For the h.c.p. the shift vectors $\mathbf{S}$ and $-\mathbf{S}$ associated with growth faults are indicated. For the f.c.c. the growth fault shown involves a change from translation vector $\mathbf{R}_1$ to $\mathbf{R}_2$. The shift vectors $\mathbf{S}_1$ and $\mathbf{S}_2$ associated with deformation faults for the two structure variants are also indicated.

intensity distribution can be derived readily from the general expressions (7) or (9). For most purposes the modifications of the structure at the fault for the h.c.p. stacking sequence can be ignored.

As a simple example we consider the case of growth faults for the f.c.c. structure. For the two types of layer $F_1=F_2$, but $\mathbf{R}_1$ and $\mathbf{R}_2$ differ, $\mathbf{S}=0$ and $\alpha_{12}=\alpha_{21}=\alpha$; $g_1=g_2=\frac{1}{2}$. Writing for convenience $\exp \mathbf{R}_1$ for $\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}_1\}$ and $(\mathbf{R}_1)$ for $[1-(1-\alpha)\exp\{2\pi i\mathbf{u}\,.\,\mathbf{R}_1\}]$, the expression (9) becomes

$$I/N=\frac{F}{2(\mathbf{R}_1)}\left[F+\frac{\alpha\exp\mathbf{R}_1}{(\mathbf{R}_2)}\left[F+\frac{\alpha\exp\mathbf{R}_2}{(\mathbf{R}_1)}\left[F+\ldots\right]\right]\right]+\frac{F}{2(\mathbf{R}_2)}\left[F+\frac{\alpha\exp\mathbf{R}_2}{(\mathbf{R}_1)}\left[F+\frac{\alpha\exp\mathbf{R}_1}{(\mathbf{R}_2)}\left[F+\ldots\right]\right]\right]+\text{c.c.}-F^2,$$

which simplifies to

$$\begin{aligned}I(\mathbf{u})/N=&\alpha(1-\alpha)F^2[1-\cos 2\pi\mathbf{u}\,.\,(\mathbf{R}_1-\mathbf{R}_2)]\\&\times[2-4\alpha+3\alpha^2-(1-\alpha)^2\{2\cos 2\pi\mathbf{u}\,.\,\mathbf{R}_1\\&+2\cos 2\pi\mathbf{u}\,.\,\mathbf{R}_2-\cos 2\pi\mathbf{u}\,.\,(\mathbf{R}_1-\mathbf{R}_2)\}\\&+(1-2\alpha)\cos 2\pi\mathbf{u}\,.\,(\mathbf{R}_1+\mathbf{R}_2)]^{-1}.\end{aligned}\tag{16}$$

In terms of rectangular axes, with a c axis perpendicular to the layers, $\mathbf{R}_1+\mathbf{R}_2=2\mathbf{a}/3$ and $R_1+R_2=2c$. The periodicity of the individual layers confines the intensities to the lines for which $\mathbf{u}\,.\,\mathbf{a}$ is integral. If $\mathbf{u}\,.\,\mathbf{a}=3n$ the intensity is zero except for the sharp peaks for $\mathbf{u}\,.\,\mathbf{c}$ integral. For $\mathbf{u}\,.\,\mathbf{a}=3n\pm1$, there are intensity maxima for $\mathbf{u}\,.\,\mathbf{c}=m\pm\frac{1}{3}$ for integral m. The height of the maxima is proportional to $(1-\alpha)/\alpha$.

The other types of faulting in close-packed structures may be treated with equal facility to give results similar to those obtained by other methods. The main advantage of the present approach for this type of problem seems to be that it is easier to define fault vectors, with or without additions and subtractions at the fault, than to construct 'probability trees' or the equivalent. For the more exotic type of fault systems occurring in more complicated structures the appropriate simplification of the more general results is not usually difficult to determine.

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