because of the creation, in the common polytype, of edge dislocations of Burger's vector, (**a**/3+2**b**/3) or (2**a**/3+**b**/3) or an integral multiple of these, at regular intervals. The formation of a lower polytype is governed by potential energy considerations while that of the long-period structure (for which the difference of energy is vanishingly small) is determined by the vibration entropy. Since it occurs more commonly than all other polytypes, the type 4*H* is believed to possess the minimum free energy. The higher polytypes of cadmium iodide are supposed to be formed by the introduction of stacking faults resulting from partial dislocations. The heating of a high polytype will help the partial dislocations to diffuse out, as proposed above, the polytype thus reverting to the parent 4*H* structure. Such a process will be favoured thermodynamically, since the system will always tend to adopt a configuration of minimum free energy. Thus the observed transformation of the type 46*H* (Fig. 2) to 4*H* (Fig. 4) is explained. Such a transformation cannot be understood on the screw dislocation theory of polytypism (Frank, 1951) according to which very stable polytypes should be formed by the mechanism of spiral growth.

Studies carried out on other cadmium iodide crystals have revealed that the process of transformation from a higher to a lower polytype is a gradual one. For instance, on heating a polytype 32*H*, the intensity of its diffraction spots changed, showing that the polytype remained of the type 32*H* without any change in its unit-cell dimensions, but the sequence of layers along the *c* dimension changed. Also, the change in intensity was such that the intense spots occurred at the positions of spots of the common type 4*H*. On heating again for the same time and at the same temperature, the intensity sequence changed further, but the spacing between the diffraction spots still remained the same, showing that the polytype was still 32*H*. The intensity sequence now resembled still more that of the type 4*H*. On further heating, the polytype ultimately changed to the common polytype 4*H* (photographs not reproduced). It follows that not only do the partial dislocations diffuse out gradually from the crystal, but they do so with regularity.

The above observations clearly bring out the important role played by stacking faults in the formation of polytypes. The detailed experimental results will be presented elsewhere in due course.

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Bragg Reflexion Intensity Distributions of Small Distorted Crystals with Stacking Faults

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General equations (within the limitations of the geometrical theory) are given describing the intensity distributions of Bragg reflexions of small distorted crystals with stacking faults. In these equations functions occur representing the stacking-fault densities, the form of the average coherently scattering region and the distribution of the relative translations of the unit cells due to the distortions apart from a lattice vector. The equations describing the intensity distribution of a Debye–Scherrer line can be inverted and give then the stacking-fault density, the distribution of the relative translations of the unit cells, and the form function of the average coherently scattering region in the direction perpendicular to the reflecting planes. A general method is given for separating the three effects: distortions, stacking faults and the size of the average coherently scattering region.

Introduction

In the analysis of the structure of distorted crystalline materials by X-ray diffraction we distinguish three different types of effects, due to crystallite size, random translations of the unit cells from their 'ideal' positions, and stacking faults.

The work of Warren & Avergach (1952) for the case in which crystallite size effects occur in combination with the random shifts of unit cells is very well known. The results of Warren & Averbach hold when the distortions of the material are not too large. For a correct interpretation of the diffraction intensity distributions in the case of larger distortions it is necessary to introduce the repartition function $\mathscr{P}(\mathbf{x})$ for the material, as described in a previous paper (La Fleur, 1969) for the case of crystals without stacking faults.

The repartition function $\mathscr{P}(\mathbf{x})$ is defined as the probability density of finding a unit cell at a distance $\mathbf{x}$ from all other unit cells in the material. The use of the function $\mathscr{P}(\mathbf{x})$ is relevant only in the case without stacking faults, in which all unit cells can be considered to be identical. It is necessary therefore to extend the calculations of the previous paper (La Fleur, 1969) in order to include also the stacking-fault effect. This is the subject of the present paper. The problem of separating the three effects will be discussed also.

To that end we need a general description of the stacking-fault effect. [Descriptions in terms of difference equations are given, for a number of particular types of structure, *e.g.* by Warren (1968)]. A stacking fault is a uniform translation of the atoms at one side of a plane with respect to the atoms at the other side of that plane. The plane is called the glide plane of the stacking fault and the translation is parallel to it. The unit cells of the crystal that are intersected by such a glide plane have a structure factor different from that of the other unit cells in the crystal. We assume that various types of stacking fault occur in the material and denote a certain type of stacking fault by the subscript p. The structure factor of a normal unit cell is indicated by f_o and that of the unit cells intersected by the glide plane of a stacking fault of type p is indicated by f_p.

The perpendicular to the glide plane of a stacking fault of type p is denoted by $\mathbf{x}_p'$ ($|\mathbf{x}_p'|=1$). One of the two vectors $\mathbf{x}_p'$ and $-\mathbf{x}_p'$ is chosen as the characteristic direction of the glide plane and denoted by $\mathbf{x}_p$. The translation of the atoms by the stacking fault of type p is denoted by $\Delta\mathbf{u}_p$. It is defined in such a way, that it fulfils the following condition. Consider the vector $\mathbf{x}$ pointing from a unit cell to another one and suppose that $\mathbf{x}$ is intersected by a glide plane of a stacking fault of type p. This distance vector $\mathbf{x}$ is given by

$$\mathbf{x}=\mathbf{a}+\Delta\mathbf{u}_p \quad \text{if} \quad (\mathbf{x}\,.\,\mathbf{x}_p) > 0\,,$$

$$\text{and} \quad \mathbf{x}=\mathbf{a}-\Delta\mathbf{u}_p \quad \text{if} \quad (\mathbf{x}\,.\,\mathbf{x}_p) < 0\,.$$

Here $\mathbf{a}$ is the distance vector between the same two unit cells, but in the absence of the stacking fault considered. By definition $\Delta\mathbf{u}_o=0$. In the same way the position of a unit cell intersected by the glide plane of a stacking fault is defined: $\mathbf{b}+\frac{1}{2}\Delta\mathbf{u}_p$. Here $\mathbf{b}$ is the position vector of the same unit cell if the stacking fault would be absent. In the following we call a unit cell that is intersected by a stacking fault of type p a unit cell of type p. (Each type of stacking fault is assumed to 'produce' only one new type of unit cell.)

It is assumed in the following, that, in addition to the translations due to the stacking faults, the unit cells are also translated with respect to each other owing to random distortions. Rotations and distortions of the individual unit cells will be neglected, except, of course, the distortion due to the stacking faults.

The characterization of the random distortions must be adapted to the case in which stacking faults are present. Instead of the repartition function $\mathscr{P}(\mathbf{x})$ the quantity $N_{pp'}(\mathbf{x})\mathscr{P}_{pp'}(\mathbf{x})\mathrm{d}\mathbf{x}$ is introduced. This is the number of unit cells of type p' that is found at a distance between $\mathbf{x}$ and $\mathbf{x}+\mathrm{d}\mathbf{x}$ from all unit cells of type p. Let us introduce also a lattice with lattice points $\mathbf{x}_m$ and primitive translation basis vectors $\mathbf{e}_i$ ($i=1, 2, 3$). Then the vector $\mathbf{x}$ is given by $\mathbf{x}=\mathbf{x}_m+\Delta\mathbf{x}$, where $\mathbf{x}_m$ is chosen so that

$$(\mathbf{e}_i\,.\,\Delta\mathbf{x}) \le \tfrac{1}{2}|\mathbf{e}_i|^2 \quad (i=1, 2, 3)\,. \tag{1}$$

In the above definition the function $N_{pp'}(\mathbf{x})$ is a slowly varying function of $\mathbf{x}$, except for $\mathbf{x}=0$. It is chosen such that for all $\mathbf{x}_m$:

$$\int N_{pp'}(\mathbf{x})\mathscr{P}_{pp'}(\mathbf{x})\mathrm{d}\mathbf{x} \simeq N_{pp'}(\mathbf{x}_m)\int \mathscr{P}_{pp'}(\mathbf{x})\mathrm{d}\mathbf{x}=N_{pp'}(\mathbf{x}_m).$$

The limits of integration are determined by

$$|\{\mathbf{e}_i\,.\,(\mathbf{x}-\mathbf{x}_m)\}| \le \tfrac{1}{2}|\mathbf{e}_i|^2\,. \tag{2}$$

Thus $N_{pp'}(\mathbf{x}_m)$ is equal to the number of unit cells of type p' that can be found at a distance between $\mathbf{x}_m$ and $\mathbf{x}_m+\Delta\mathbf{x}'$ from all unit cells of type p, where $\Delta\mathbf{x}'$ indicates the boundaries of the cell defined by relationship (1). At $\mathbf{x}=0$ the function $N_{pp'}(\mathbf{x})$ possesses a discontinuity, since by definition

$$N_{pp'}(0)=0 \quad \text{if} \quad p \ne p'\,, \tag{3a}$$

and

$$N_{pp'}(\mathbf{x}) \ne 0 \quad \text{if} \quad p \ne p' \text{ and } \mathbf{x} \ne 0 \tag{3b}$$

when the material contains stacking faults.

In the following, we will neglect the effects due to the intersection of two glide planes of stacking faults of different type.

Derivation of the equations

The diffraction intensity distribution of a distorted crystalline material containing stacking faults is calculated as follows, within the limitations of the geometric theory. The structure factor of the material is

$$F=\sum_p \sum_{n=n_p} f_p \exp\{2\pi i\mathbf{s}\,.\,(\mathbf{u}_n+\Delta\mathbf{u}_n+\tfrac{1}{2}\Delta\mathbf{u}_p + \sum_p a_{p,\,n}\Delta\mathbf{u}_p)\}\,, \tag{4}$$

in which the symbols represent the following:

$\mathbf{s}$: reciprocal space coordinate.

n: set of three integers n_1, n_2, n_3, numbering the unit cells.

$\mathbf{u}_n$: position of the nth unit cell in an ideal, undistorted crystal with respect to a certain origin.

$\Delta\mathbf{u}_n$: translation of the nth unit cell due to the random distortions.

$\Delta\mathbf{u}_p$: translation of a unit cell when a glide plane of a stacking fault of type p occurs between the origin and the nth unit cell.

$a_{p,\,n}$: number of glide planes of type p between the origin and the nth unit cell.

n_p: set of indexes n for the unit cells of type p.

The summation in equation (4) is taken over all p and all n_p. The corresponding intensity distribution $I(\mathbf{s})$ is

$$I(\mathbf{s})=F(\mathbf{s})F(\mathbf{s})^*=$$

$$\sum_{pp'}\sum_{\substack{n'=n'_{p'}\\ n=n_p}} f_pf^*_{p'}\exp\,[2\pi i\mathbf{s}\,.\,\{\mathbf{u}_n-\mathbf{u}_{n'}+\Delta\mathbf{u}_n-\Delta\mathbf{u}_{n'}$$
$$+\tfrac{1}{2}(\Delta\mathbf{u}_p-\Delta\mathbf{u}_{p'})+\sum_p(a_{p,\,n}-a_{p,\,n'})\Delta\mathbf{u}_p\}]\,. \quad (5)$$

The sum of the translations $\mathbf{u}_n$, $-\mathbf{u}_{n'}$, $\Delta\mathbf{u}_n$, etc., occurring in the exponential of equation (5) is replaced by $\mathbf{x}=\mathbf{x}_m+\Delta\mathbf{x}$, where $\mathbf{x}$, $\mathbf{x}_m$ and $\Delta\mathbf{x}$ are defined as in the introduction. In the same time $P_{pp'}(\mathbf{x}_m;\,\Delta\mathbf{x}_k)$ is put for the number of unit cells of type p' that are at a distance $\mathbf{x}_m+\Delta\mathbf{x}_k$ from all unit cells of type p in the material. Thus we can replace equation (5) by

$$I(\mathbf{s})=\sum_{pp'}f_pf^*_{p'}\sum_{m,k}P_{pp'}(\mathbf{x}_m;\,\Delta\mathbf{x}_k)$$
$$\times\exp\,\{2\pi i\mathbf{s}\,.\,(\mathbf{x}_m+\Delta\mathbf{x}_k)\}\,. \quad (6)$$

In a corresponding integral form this equation becomes

$$I(\mathbf{s})=\sum_{pp'}f_pf^*_{p'}\sum_m\int_{-\infty}^{+\infty}\Phi_{pp'}(\mathbf{x}_m;\,\Delta\mathbf{x})$$
$$\times\exp\,(2\pi i\mathbf{s}\,.\,(\mathbf{x}_m+\Delta\mathbf{x})\}\mathrm{d}(\Delta\mathbf{x})\,. \quad (7)$$

In this equation $\Phi_{pp'}(\mathbf{x}_m;\,\Delta\mathbf{x})\mathrm{d}(\Delta\mathbf{x})$ is the number of unit cells of type p and p' that is found at a distance between $\mathbf{x}_m+\Delta\mathbf{x}$ and $\mathbf{x}_m+\Delta\mathbf{x}+\mathrm{d}(\Delta\mathbf{x})$ from each other. By the definition of $\Delta\mathbf{x}$ we may put

$$\Phi_{pp'}(\mathbf{x}_m;\,\Delta\mathbf{x})=0,$$

when

$$|(\mathbf{e}_i\,.\,\Delta\mathbf{x})|\le|\mathbf{e}_i|^2;\ (i=1,\,2\text{ or }3)\,. \quad (8)$$

Comparing the definitions of $\Phi_{pp'}(\mathbf{x}_m;\Delta\mathbf{x})$ and $N_{pp'}(\mathbf{x})\mathscr{P}_{pp'}(\mathbf{x})$, we observe that

$$\sum_m\Phi_{pp'}(\mathbf{x}_m;\,\Delta\mathbf{x})=N_{pp'}(\mathbf{x})\mathscr{P}_{pp'}(\mathbf{x})\,. \quad (9)$$

Equation (9) can be substituted into equation (7) to give

$$I(\mathbf{s})=\sum_{pp'}f_pf^*_{p'}\int_{-\infty}^{+\infty}N_{pp'}(\mathbf{x})\mathscr{P}_{pp'}(\mathbf{x})\exp\,(2\pi i\mathbf{s}\,.\,\mathbf{x})\mathrm{d}\mathbf{x}\,. \quad (10)$$

Apart from the translation $\frac{1}{2}\Delta\mathbf{u}_p$ due to a stacking fault the relative translations of the unit cells due to distortions that are first neighbours are very small. Therefore we can equate $\mathscr{P}_{pp'}(\mathbf{x})$ in good approximation to

$$\mathscr{P}_{pp'}(\mathbf{x})=\mathscr{P}_{oo}(\mathbf{x}\pm\tfrac{1}{2}\Delta\mathbf{u}_p\pm\tfrac{1}{2}\Delta\mathbf{u}_{p'})$$

when

$$(\mathbf{x}\,.\,\mathbf{x}_p)\neq0$$
$$(\mathbf{x}\,.\,\mathbf{x}_{p'})\neq0\,.$$

$$\mathscr{P}_{pp'}(\mathbf{x})=\mathscr{P}_{oo}(\mathbf{x})$$

when

$$(\mathbf{x}\,.\,\mathbf{x}_p)=(\mathbf{x}\,.\,\mathbf{x}_{p'})=0\,. \quad (11)$$

The + sign for $\Delta\mathbf{u}_p$ applies, when $(\mathbf{x}\,.\,\mathbf{x}_p)<0$, and the − sign applies when $(\mathbf{x}\,.\,\mathbf{x}_p)>0$. The same is true for the expressions in p'.

We substitute this set of equations in equation (10). For the ease of writing we introduce at the same time the function $G_{pp'}(\mathbf{x};\,\mathbf{s})$. This function is defined as

$$G_{pp'}(\mathbf{x};\,\mathbf{s})=\exp\,\{\pi i\mathbf{s}\,.\,(\pm\Delta\mathbf{u}_p\pm\Delta\mathbf{u}_{p'})\}$$

when

$$(\mathbf{x}\,.\,\mathbf{x}_p)\neq0$$
$$(\mathbf{x}\,.\,\mathbf{x}_{p'})\neq0$$

$$G_{pp'}(\mathbf{x};\,\mathbf{s})=1$$

when

$$(\mathbf{x}\,.\,\mathbf{x}_p)=(\mathbf{x}\,.\,\mathbf{x}_{p'})=0 \quad (12)$$

with the same sign convention as (11).

Since $N_{pp'}(\mathbf{x})$ varies slowly with $\mathbf{x}(\mathbf{x}\neq0)$, then equation (10) becomes

$$I(\mathbf{s})=\sum_{pp'}f_pf^*_{p'}\int_{-\infty}^{+\infty}G_{pp'}(\mathbf{x};\,\mathbf{s})N_{pp'}(\mathbf{x})\mathscr{P}_{oo}(\mathbf{x})$$
$$\times\exp\,(2\pi i\mathbf{s}\,.\,\mathbf{x})\mathrm{d}\mathbf{x}\,. \quad (13)$$

This equation can be treated in the same way as equation (7) in the previous paper (La Fleur, 1969). At first $\mathscr{P}_{oo}(\mathbf{x})$ is expressed as

$$\mathscr{P}_{oo}(\mathbf{x})=\sum_m\,[C'(\mathbf{x}_m)\varphi'(\mathbf{x}_m;\,\Delta\mathbf{x})+v^{-1}\{1-C'(\mathbf{x})\}]_{\text{[illegible]}} \quad (14)$$

where $C'(\mathbf{x})$ is chosen such that

$$\varphi'\{\mathbf{x}_m;\,\tfrac{1}{2}(\mathbf{e}_1,\,\mathbf{e}_2,\,\mathbf{e}_3)\}=0 \quad (15)$$

and

$$\int_{|(\mathbf{e}_i\,.\,\Delta\mathbf{x})|\le\frac{1}{2}|\mathbf{e}_i|^2}\varphi'(\mathbf{x}_m;\,\Delta\mathbf{x})\mathrm{d}(\Delta\mathbf{x})=1. \quad (16)$$

In these equations v is the volume of a unit cell of the lattice. Let us introduce also the functions $\varphi(\mathbf{x};\,\Delta\mathbf{x})$ and $C(\mathbf{x})$ varying slowly with $\mathbf{x}$. For $\mathbf{x}=\mathbf{x}_m$ these functions have the values

$$C(\mathbf{x}_m)=C'(\mathbf{x}_m) \quad (17)$$

$$\varphi(\mathbf{x}_m;\,\Delta\mathbf{x})=\varphi'(\mathbf{x}_m;\,\Delta\mathbf{x})\,. \quad (18)$$

By means of equations (14), (17) and (18), equation (13) is written

$$I(\mathbf{s})=I_a(\mathbf{s})+I_b(\mathbf{s})\,. \quad (19)$$

Where

$$I_a(\mathbf{s})=\sum_{pp'}f_pf^*_{p'}\int_{-\infty}^{+\infty}\sum_m\delta(\mathbf{x}-\mathbf{x}_m)\,A_{pp'}(\mathbf{x};\,\mathbf{s})$$
$$\times\exp\,(2\pi i\mathbf{s}\,.\,\mathbf{x})\mathrm{d}\mathbf{x} \quad (20)$$

with

$$A_{pp'}(\mathbf{x};\,\mathbf{s}) = C(\mathbf{x})G_{pp'}(\mathbf{x};\,\mathbf{s})N_{pp'}(\mathbf{x}) \times \int_{-\infty}^{\infty} \varphi(\mathbf{x};\,\Delta\mathbf{x}) \exp(2\pi i\mathbf{s}\,.\,\Delta\mathbf{x})\mathrm{d}(\Delta\mathbf{x})\,. \quad (21)$$

$I_b(\mathbf{s})$ is the remaining term, corresponding to the second term $v^{-1}\{1-C(\mathbf{x})\{$ in equation (14) for $\mathscr{P}_{oo}(\mathbf{x})$.

The first term $I_a(\mathbf{s})$ in equation (19) becomes then

$$\begin{aligned} I_a(\mathbf{s}) = {} & \sum_{pp'} f_p f^*_{p'} \int_{-\infty}^{+\infty} A_{pp'}(\mathbf{x};\,\mathbf{s}) \sum_m \delta(\mathbf{x}-\mathbf{x}_m) \\ & \times \exp(2\pi i\mathbf{s}\,.\,\mathbf{x})\mathrm{d}\mathbf{x} = \sum_{pp'} f_p f^*_{p'} \int_{-\infty}^{+\infty} A_{pp'}(\mathbf{x};\,\mathbf{s}) \\ & \times \exp(2\pi i\mathbf{s}\,.\,\mathbf{x})\mathrm{d}\mathbf{x} * \int_{-\infty}^{+\infty} \sum_m \delta(\mathbf{x}-\mathbf{x}_m) \\ & \times \exp(2\pi i\mathbf{s}\,.\,\mathbf{x})\mathrm{d}\mathbf{x} = \sum_{pp'} f_p f^*_{p'} \int_{-\infty}^{+\infty} A_{pp'}(\mathbf{x};\,\mathbf{s}) \\ & \times \exp(2\pi i\mathbf{s}\,.\,\mathbf{x})\mathrm{d}\mathbf{x} * \sum \delta(\mathbf{s}-\mathbf{s}_l) = \\ & \sum_l \sum_{pp} f_p f^*_{p'} \int_{-\infty}^{+\infty} A_{pp'}(\mathbf{x};\,\mathbf{s}_l) \exp\{2\pi i\mathbf{x}\,.\,(\mathbf{s}-\mathbf{s}_l)\}\mathrm{d}\mathbf{x}\,. \end{aligned} \quad (22)$$

Here $*$ means convolution integral of the quantities at both sides of the sign. Furthermore $\mathbf{s}_l$ is the lth point of the reciprocal lattice ($l=l_1, l_2, l_3$), chosen such that

$$(\mathbf{x}_m\,.\,\mathbf{s}_l) \text{ is an integer}\,. \quad (23)$$

In equation (22) the terms in the summation over l are identified with the intensity distributions of the singular spots of a diffraction pattern $I_l(\mathbf{s}-\mathbf{s}_l)$, where

$$I(\mathbf{s}) = \sum_l I_l(\mathbf{s}-\mathbf{s}_l)\,. \quad (24)$$

The result of this identification is:

$$I(\mathbf{s}-\mathbf{s}_l) = \sum_{pp'} f_p f^*_{p'} \int_{-\infty}^{+\infty} A_{pp'}(\mathbf{x};\,\mathbf{s}_l) \times \exp(2\pi i\mathbf{x}\,.\,(\mathbf{s}-\mathbf{s}_l)\}\mathrm{d}\mathbf{x}\,. \quad (25)$$

The identification makes sense when the diffraction pattern consists of (broadened) spots around the points $\mathbf{s}_l$, that can be separated from each other, so $I_l(\mathbf{s}-\mathbf{s}_l)$ must decrease sufficiently rapidly with $|\mathbf{s}-\mathbf{s}_l|$. This implies that $A_{pp'}(\mathbf{x};\,\mathbf{s}_l)$ varies sufficiently slowly with $\mathbf{x}$. However, $A_{pp'}(\mathbf{x};\,\mathbf{s}_l)$ contains the function $G_{pp'}(\mathbf{x};\,\mathbf{s}_l)$. This is a step function of $\mathbf{x}$ unless $p=p'=0$. Therefore $A_{pp'}(\mathbf{x};\,\mathbf{s}_l)$ only can be a slowly varying function of $\mathbf{x}$, when $N_{pp'}(\mathbf{x})$ ($p, p' \neq 0$) is sufficiently small compared with $N_{oo}(\mathbf{x})$; in addition $\varphi(\mathbf{x};\,\Delta\mathbf{x})$ and $C(\mathbf{x})$ must vary slowly with $\mathbf{x}$. Thus the stacking-fault density is relatively small when the diffraction pattern consists of discrete (broadened) spots around $\mathbf{s}_l$.

The second term of equation (19): $I_b(\mathbf{s})$ can be shown to give a small angle effect, described by the δ function $\delta(\mathbf{s})$, if it is combined with the term for $l=(0, 0, 0)$ in the summation over l in equation (22).

In the case of a crystal without stacking faults equation (25) reduces to equation (31) of the previous paper. In that paper $C(\mathbf{x})$ was called the form function of the average coherently scattering region. It is seen, that the meaning of $C(\mathbf{x})$ in the case of a crystal with stacking faults is the same as that in the case of a crystal without stacking faults.

The function $C(\mathbf{x})$ decreases when the relative translations (assumed to be at random) of the unit cells due to the distortions increase. Therefore the size of the average coherently scattering region decreases by increasing distortions. The stacking faults also 'produce' relative translations of the unit cells and consequently the size of the average coherently scattering region decreases when the stacking-fault density increases.

We have to realize that $C(\mathbf{x})$, in the case of large distortions and in the case of relatively large stacking-fault densities, is only a characteristic of $\mathscr{P}_{oo}(\mathbf{x})$. Furthermore the function $C(\mathbf{x})$ depends in these cases on the choice of the primitive translation basis vectors of the lattice.

The intensity distribution of a Debye–Scherrer line can be derived from equation (25) in the same way as it is derived for the case where there are no stacking faults.

$$I_l(\mathbf{s}_0) = \sum_{pp'} f_p f^*_{p'} \int_{-\infty}^{+\infty} G_{pp'}(t;\,s_l)N_{pp'}(t)C(t) \times \exp(2\pi i s_0 t)\mathrm{d}t \int_{-\infty}^{+\infty} \varphi(t;\,L) \exp(2\pi i s_l L)\mathrm{d}L\,. \quad (26)$$

In this formula s_0 is equal to the projection of the reciprocal lattice coordinate $\mathbf{s}-\mathbf{s}_l$ on the direction of $\mathbf{s}_l$. The parameter t is the modulus of a vector perpendicular to the reflecting planes; the modulus of $\mathbf{s}_l$ is denoted by s_l. The symbols $G_{pp'}(t;\,s_l)$, $N_{pp'}(t)$ and $C(t)$ are used for $G_{pp'}(\mathbf{x};\,\mathbf{s}_l)$, $N_{pp'}(\mathbf{x})$ and $C(\mathbf{x})$ in the direction perpendicular to the reflecting planes, respectively. The parameter L is the projection of $\Delta\mathbf{x}$ on that direction. When $\varphi(\mathbf{x};\,L)$ is the projection of $\varphi(\mathbf{x};\,\Delta\mathbf{x})$ on the same direction perpendicular to the reflecting planes, we can define $\varphi(t;\,L)$ as being $\varphi(\mathbf{x};\,L)$ in that direction.

If the diffraction lines are discrete, and for $L \geq \frac{1}{2}d$ (where d is interplanar spacing), we can put $\varphi(t;\,L)=0$. We have, however, to analyse the significance of $C(t)$ and of $\varphi(t;\,L)$ when this is done. This is done by summing the intensity distributions of all orders of reflexion for one crystallographic direction.

$$I(s) = \sum I_l(s_0) = I_l(s) * \sum_l \delta(s-s_l)\,. \quad (27)$$

Here the term analogous to $I_b(\mathbf{s})$ is not included. The parameter s is used for $|\mathbf{s}|$ in the direction of $\mathbf{s}_l$. When equation (26) is substituted into equation (27) we get

$$I(s)=$$

$$\sum_l \delta(s-s_l) * \sum_{pp'} \int_{-\infty}^{+\infty} N_{pp'}(t)C(t)G_{pp'}(t;\, s_l)$$

$$\times \exp\,(2\pi i s_0 t)\mathrm{d}t \int_{-\infty}^{+\infty} \varphi(t;\, L) \exp\,(2\pi i s_l L)\mathrm{d}L$$

$$= \sum_{pp'} f_p f^*_{p'} \int_{-\infty}^{+\infty} \delta(t-t_n) N_{pp'}(t)C(t)G_{pp'}(t;\, s_l)$$

$$\times \exp\,(2\pi i s_0 t)\mathrm{d}t \int_{-\infty}^{+\infty} \varphi(t;\, L) \exp\,(2\pi i s_l L)\mathrm{d}L \quad (28)$$

where $t_n = nd$ and n is an integer. If we include the term analogous to $I_b(\mathbf{s})$, we may write for equation (28)

$$I(s) = \sum_{pp'} f_p f^*_{p'} \int_{-\infty}^{+\infty} N_{pp'}(t) G_{pp'}(t;\, s) \times \mathscr{P}_{oo}(t) \exp\,(2\pi i s t)\mathrm{d}t\,. \quad (29)$$

The function $\mathscr{P}_{oo}(t)$ is a repartition function

$$\mathscr{P}_{oo}(t) = \sum_n C(t_n)\varphi(t_n;\, t-t_n) + d^{-1}\{1-C(t)\}\,. \quad (30)$$

From equation (30), $\mathscr{P}_{oo}(t)$ can be written as the sum of the projections $\varphi(t_n;\, t-t_n)$ of $\varphi(\mathbf{x};\, \Delta\mathbf{x})$ times $C(t_n)$ plus the term $d^{-1}\{1-C(t)\}$. The functions $\varphi(t_n;\, t-t_n)$ do not fulfil the condition $\varphi(t_n;\, t-t_n)=0$ for $|t-t_n| \geq \frac{1}{2}d$. However, it can be shown, that we can reformulate $\mathscr{P}_{oo}(t)$, without changing the result for the intensity distribution $I_n(s_0)$, as

$$\mathscr{P}_{oo}(t) = \sum_n C''(t_n)\varphi''(t_n;\, t-t_n) + d^{-1}\{1-C''(t)\}\,. \quad (31)$$

With

$$\varphi''(t_n;\, t-t_n) = 0 \quad \text{when} \quad t-t_n \geq \tfrac{1}{2}d \quad (32)$$

and

$$\int_{t_n-\frac{1}{2}d}^{t_n+\frac{1}{2}d} \varphi''(t_n;\, t-t_n)\mathrm{d}t = 1\,. \quad (33)$$

When we replace in equation (26) $\varphi(t;\, L)$ and $C(t)$ with $\varphi''(t;\, L)$ and $C''(t)$, the result for $I_n(s_0)$ remains unchanged. The function $\varphi''(t_n;\, t-t_n)$ is approximately equal to the projection of $\varphi(t;\, \Delta\mathbf{x})$ in the direction perpendicular to the reflecting planes if the reflecting planes are spanned up by two of the three primitive translation vectors, or when $\varphi(\mathbf{x};\, \Delta\mathbf{x})$ is a very sharp function of $\Delta\mathbf{x}$. The unprimed quantities cannot be derived uniquely from the primed ones, so the primed quantities can only be determined from a powder diagram unless a model of the distortions is assumed. (For ease of writing, the primes are omitted in the following.)

Inversion of the equations

For the analysis of the structure of distorted crystalline materials it is of interest to invert equation (26). Furthermore the effects of distortion, size and stacking faults have to be separated. Below, a method is given for the separation of the stacking-fault effect from both the size and the distortion effects. When this separation is carried out, one can proceed by means of the known methods for the separation of the size effect from the distortion effect. (Warren & Averbach, 1952; La Fleur & Koopmans, 1968.) We confine ourselves to the powder diagram.

Let us put

$$\int_{-\infty}^{+\infty} \varphi(t;\, L) \exp\,(2\pi i s_l L)\mathrm{d}L = a(t;\, s_l) \quad (34)$$

The Fourier transform of $I_l(s_0)$: $A(t;\, s_l)$ is equal to:

$$A(t;\, s_l) = \sum_{pp'} f_p f^*_{p'}\; C(t) N_{pp'}(t) G_{pp'}(t;\, s_l) a(t;\, s_l)\,. \quad (35)$$

The stacking-fault density is necessarily relatively small if the diffraction lines are discrete. Therefore $N_{pp'}(t)$ $(p, p' \neq 0;\, t>0)$ can be neglected in comparison with $N_{op}(t)$ and $N_{po}(t)$. Thus, we have

$$N = N_{oo}(t) + \sum_{p\neq o} N_{op}(t) = N_{oo}(-t) + \sum_{p\neq o} N_{op}(-t)\,. \quad (36)$$

It follows from the definition of $N_{op}(t)$ and $N_{po}(t)$, that:

$$N_{op}(t) = N_{po}(-t) \quad (37)$$

and, combining equations (36) and (37), we find:

$$N_{op}(t) = N_{po}(t)\,. \quad (38)$$

By the definition of $G_{pp'}(t;\, s_l)$ we may write

$$G_{pp'}(t;\, s_l) = G_{p'p}(t;\, s_l)\,. \quad (39)$$

Equations (39) and (37) are substituted into equation (35); $N_{pp'}(t)$ $(p, p' \neq 0)$ is neglected. The result is

$$A(t;\, s_l) = f_o f^*_o N_{oo}(t) C(t) a(t;\, s_l)$$

$$+ \sum_{p\neq o} \{2\mathrm{Re}\, f_o f^*_p\} G_{op}(t;\, s_l) N_{op}(t) C(t) a(t;\, s_l)\,. \quad (40)$$

We will write down the imaginary part and the real part of equation (40) separately. To that end we denote the real part of $A(t;\, s_l)$, $a(t;\, s_l)$ and $G_{op}(t;\, s_l)$ with: $A^{\mathrm{re}}(t;\, s_l)$, $a^{\mathrm{re}}(t;\, s_l)$ and $G^{\mathrm{re}}_{op}(t;\, s_l)$ respectively. The corresponding imaginary parts are indicated with the superscript 'im'. We denote $f_o f^*_o$ by F_o, $\{2\mathrm{Re}\, f_o f^*_p\}$ $G^{\mathrm{re}}_{op}(t;\, s_l)$ by F^{re}_p, and $\{2\mathrm{Re}\, f_o f^*_p\} G^{\mathrm{im}}_{op}(t;s_l)$ by F^{im}_p. We find then for the real and imaginary parts of equation (40), respectively:

$$A^{\mathrm{re}}(t;\, s_l) = F_o\{N - \sum_{p\neq o} N_{op}(t)\} C(t) a^{\mathrm{re}}(t;\, s_l)$$

$$+ \sum_{p\neq o} F^{\mathrm{re}}_p N_{op}(t) C(t) a^{\mathrm{re}}(t;\, s_l)$$

$$- \sum_{p\neq o} F^{\mathrm{im}}_p N_{op}(t) C(t) a^{\mathrm{im}}(t;\, s_l) \quad (41)$$

and

$$A^{\mathrm{im}}(t;\, s_l) = F_o\{N - \sum_{p\neq o} N_{op}(t)\} C(t) a^{\mathrm{im}}(t;\, s_l)$$

$$+\sum_{p\neq o} F_p^{\mathrm{im}} N_{op}(t)C(t)a^{\mathrm{re}}(t;s_l)$$
$$+\sum_{p\neq o} F_p^{\mathrm{re}} N_{op}(t)C(t)a^{\mathrm{im}}(t;s_l)\,. \qquad (42)$$

The above equations hold when an arbitrary number of different types of stacking faults occur in the material. Each new combination of the vectors $\mathbf{x}_p$ and $\Delta\mathbf{u}_p$ could characterize a new type of stacking fault. Let us assume now that for each glide plane direction $\mathbf{x}_p$ only one type of stacking fault occurs. This assumption is not strictly necessary, but it simplifies the further calculations. The set of all stacking faults with glide plane directions $\mathbf{x}_p = S\mathbf{x}_{p'}$ (where S is any point group symmetry operation of the crystals) could be called the set of stacking faults that are equivalent by the symmetry of the structure. Let us assume also that there exists only one of such a set of stacking faults in the crystalline material. This assumption simplifies further the calculations, but also is not strictly necessary.

For a polycrystalline material that is distorted at random, we may assume (in view of the above restrictions)

$$N_{op}(\gamma\mathbf{x}_p) = N_{op'}(\gamma\mathbf{x}_{p'}) \qquad (43)$$

if $p\neq 0$ and $p'\neq 0$ and if γ is any real parameter ($|\mathbf{x}_p| = |\mathbf{x}_{p'}| = 1$). This means that the number of unit cells of type p that are at a distance $\mathbf{x}_p$ from all unit cells of type o is equal to the number of unit cells of type p' that are at a distance $\mathbf{x}_{p'}$ from all unit cells of type o in the material.

Since we can neglect all $N_{pp'}(\mathbf{x})$ with $p, p'\neq 0$, the quantity $N_{op'}(\mathbf{x})$ is approximately constant for $\mathbf{x}\neq 0$. In view of equation (43) we can write

$$N^{-1}N_{op}(\mathbf{x}) = N^{-1}N_{op'}(\mathbf{x}) = \kappa\,. \qquad (44)$$

We can give an expression for κ in terms of the quotient $\{A^{\mathrm{im}}(t;s_l\}\,\{A^{\mathrm{re}}(t;s_l)\}^{-1}$ by expanding it into a power series of t:

$$\{A^{\mathrm{im}}(t;s_l)\}\,\{A^{\mathrm{re}}(t;s_l)\}^{-1} = a+bt+ct^2+\ldots \qquad (t>0)\,. \qquad (45)$$

Since

$$\lim_{t\downarrow 0} \varphi(t;L) = \delta(L) \qquad (46)$$

we have

$$\lim_{t\downarrow 0} a^{\mathrm{im}}(t;s_l) = 0\,. \qquad (47)$$

From equation (45) we get

$$\lim_{t\downarrow 0} A^{\mathrm{im}}(t;s_l)A^{\mathrm{re}}(t;s_l)^{-1} = a \qquad (48)$$

The results (47), (48) and (44) are combined with equations (41) and (42)

$$\kappa = aF_o\{aF_ok + \sum_{p\neq o}(F_p^{\mathrm{im}} - aF_p^{\mathrm{re}})\}^{-1}\,. \qquad (49)$$

Here k is the number of types of stacking faults. By the relations (48) and (49) the stacking-fault density κ is connected directly with the real and imaginary parts of the Fourier coefficients of the line profile of a Debye–Scherrer line. The dependence of the imaginary coefficients on the choice of d (or s_l) is the main objection against the use of the imaginary coefficients for the determination of stacking-fault densities. However, equations (48) and (49) are independent of that choice. These relations could be very useful therefore for the determination of the stacking-fault density.

Once the stacking-fault density κ is known, we can determine $C(t)a^{\mathrm{re}}(t;s_l)$ and $C(t)a^{\mathrm{im}}(t;s_l)$ from the Fourier coefficients of the line profile. To that end we substitute κ for $N^{-1}N_{op}(t)$ in equations (41) and (42). From this substitution it follows that

$$C(t)a^{\mathrm{re}}(t;s_l) = [\kappa \sum_{p\neq o} F_p^{\mathrm{im}}A^{\mathrm{im}}(t;s_l)$$
$$+A^{\mathrm{re}}(t;s_l)\,\{F_o(1-k\kappa)+\kappa\sum_{p\neq o}F_p^{\mathrm{re}}\}]$$
$$\times[\{F_o(1-k\kappa)+\kappa\sum_{p\neq o}F_p^{\mathrm{re}}\}^2+\kappa^2(\sum_{p\neq o}F_p^{\mathrm{im}})^2]^{-1} \qquad (50)$$

and

$$C(t)a^{\mathrm{im}}(t;s_l) = [A^{\mathrm{im}}(t;s_l)\,\{F_o(1-k\kappa)$$
$$+\kappa\sum_{p\neq o}F_p^{\mathrm{re}}\} - A^{\mathrm{re}}(t;s_l)\kappa\sum_{p\neq o}F_p^{\mathrm{im}}]$$
$$\times[\{F_o(1-k\kappa)+\kappa\sum_{p\neq o}F_p^{\mathrm{re}}\}^2+\kappa^2(\sum_{p\neq o}F_p^{\mathrm{im}})^2]^{-1}\,. \qquad (51)$$

In conclusion, we arrive at the following procedure for the separation of the size effect, the distortion effect and the stacking-fault effect. This procedure can be applied for a polycrystalline material, that is distorted at random and in which one set of stacking faults occurs, that are equivalent by the symmetry of the structure. This same approach is also justified when only one type of stacking fault occurs in the polycrystalline material.

By means of equations (48) and (49) the stacking-fault effect is separated from both the size effect and the distortion effect. One obtains the stacking-fault density κ. When κ is known, the quantities $C(t)a^{\mathrm{re}}(t;s_l)$ and $C(t)a^{\mathrm{im}}(t;s_l)$ are determined by means of equations (50) and (51). Using the latter quantities the size effect and the distortion effect can be separated with the methods of Warren & Averbach (1952) or with that of La Fleur & Koopmans (1968).

The equations can be extended to the case of more sets of equivalent types of stacking faults and to the case that more than one type of stacking fault occurs for one glide plane direction. These cases are probably exceptional in nature and the above procedure will be generally sufficient in the most common cases.

Discussion

We conclude from the foregoing that equation (25) gives a right description of the diffraction intensity distributions of small distorted crystals with stacking faults, within the limitations of the geometrical theory.

It is also restricted to the case that each type of stacking fault 'produces' only one new type of unit cell in the material.

The intensity distribution of a powder diagram line is described by equation (26) with the same limitations as for equation (25). The quantities $\varphi(t; L)$ and $C(t)$ in equation (26) can be replaced by $\varphi''(t; L)$ and $C''(t)$, chosen such that $\varphi''(t; L)=0$ for $L \geq \frac{1}{2}d$. This provides also a right description of the intensity distribution of a Debye–Scherrer line. The quantities $\varphi''(t; L)$ and $C''(t)$ can be found from the line profiles; the corresponding unprimed quantities cannot be found from a powder diagram, unless a model of the distortions is assumed.

The intensity distributions given in equations (25) and (26) are still unnormalized. When one wishes to determine the distribution of the distortions and the form function of the average coherently scattering region it is necessary to know the normalization constant to within the factor N. To find that constant, equation (26) is integrated over s_0

$$\begin{aligned}\int_{-\infty}^{+\infty} & I_l(s_0)\mathrm{d}s_0 \\ &= \int_{-\infty}^{+\infty}\mathrm{d}s_0 \sum_{pp'} f_p f_{p'}^* \int_{-\infty}^{+\infty} C(t) G_{pp'}(t; s_l) N_{pp'}(t) \\ &\times \exp(2\pi i s_0 t) \int_{-\infty}^{+\infty} \varphi(t; L) \exp(2\pi i s_l L)\mathrm{d}L \\ &= \sum_{pp'} f_p f_{p'}^* \int_{-\infty}^{+\infty} \delta(t) G_{pp'}(t) N_{pp'}(t)\mathrm{d}t \\ &\times \int_{-\infty}^{+\infty} \varphi(t; L) \exp(2\pi i s_l L)\mathrm{d}L \\ &= N_{oo}(0) f_o f_o^* + N_{11}(0) \sum_{p \neq o} 2\mathrm{Re} f_o f_p^* . \qquad (52)\end{aligned}$$

Here we used $G_{pp'}(0)=1$ and $N_{pp'}(0)=0$ if $p, p' \neq 0$. Equation (52) holds when all glide plane directions are equivalent by the symmetry of the structure, or, when $N_{op}(t)=0$ for $p \neq 0$ and $p \neq 1$. We have for these cases:

$$kN_{11}(0) = N - N_{oo}(0) . \qquad (53)$$

Where k is the number of types of stacking faults. Thus the inverse of the normalization constant is:

$$\int_{-\infty}^{+\infty} I_l(s_0)\mathrm{d}s_0 = f_o f_o^* N_{oo}(0) + \frac{N - N_{oo}(0)}{k} \sum_{p \neq o} \{2\mathrm{Re} f_o f_p^*\} . \qquad (54)$$

Once the stacking-fault density κ is known, one can calculate the normalization constant to within the factor N by means of relations (53) and (54) and the relation

$$\kappa = N^{-1} N_{11}(0) . \qquad (55)$$

A final remark should be made. In equations (44), (49), (50) and (51) we disregarded the special case, that one of the glide plane directions is perpendicular to $\mathbf{s}_n$. Then, for that type of stacking-fault, $N^{-1}N_{op}(t)$ equals zero instead of κ, and that value should be substituted into equations (41) and (42). Of course κ can be substituted for all other types of stacking faults. The equations (49), (50) and (51) can be adapted immediately by omitting F_p^{im} and F_p^{re} for that type of stacking fault.

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Crystal Measurements for Absorption Correction

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A method is described for determining, with few measurements and calculations, the bounding planes of a crystal.

The availability of computer programs for absorption correction by either the Gaussian integration or analytical methods (Ahmed, 1970) means that these corrections can be calculated for polyhedral crystals to any desired accuracy. This suggests that it may be preferable not to grind crystals into spheres, a proce-