sides of the origin is not in general the same. No explanation is offered for this lack of centro-symmetry in the diffraction pattern. It presumably belongs to the same class of phenomena as that which often leads to a gross lack of such symmetry in intensity in electron-diffraction patterns, and even, as in the present instance, of complete suppression of a layer line at one side of the origin.

Since the observation of the fine structure in the present work, a review of earlier electron-diffraction photographs has revealed traces of the same phenomenon on some of them, but to a much less marked degree. In some cases it may be deduced from the heights of the spots perpendicular to the layer lines that the resolution was not sufficient to resolve such a fine structure, but this is certainly not always true, and it seems probable that the fine structure does not usually appear even when the resolution is high enough.

If the structure were spiral this would be explained if the edges of the spiral layers were not parallel to the fibril axis, and if the structure were of the distorted circular type if the distortions were twisted along the length of the fibril.

One possible special case of the fine structure is worth noting. A reflection of configuration B from a fibril with a very small central hole would consist of a single sharp spot, flanked by two very weak spots which might either be missed or mistaken for subsidiary Laue maxima. In either case, if the sharpness of the central spot were taken to be due to the wall thickness of the fibril this parameter would be over-estimated by a factor of about two.

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Diffraction by Face-Centered Cubic Crystals Containing Extrinsic Stacking Faults

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The diffraction pattern of a face-centered cubic crystal containing an arbitrary density of extrinsic faults is derived. The derivation is subject to the restriction that the crystal be infinite with infinitely extended faults distributed at random on one set of parallel close-packed planes.

Although both extrinsic and intrinsic stacking faults shift and broaden the same Bragg reflections, there are marked differences in behavior which make them readily distinguishable. The peak shift produced by a low density of extrinsic faults is in a direction opposite to the shift produced by intrinsic faulting. At higher extrinsic fault densities the shifted reflections show two peaks: a new peak arises near the hexagonal position, moving to the twin position as the density of faulting approaches unity. The broadening is asymmetric at all fault densities.

Introduction

A face-centered cubic crystal, considered as a layer structure produced by the appropriate stacking of close-packed (111) planes, can contain three essentially different types of stacking error (Read, 1953):

(1) Intrinsic fault, corresponding to the removal of a close-packed plane from the perfect crystal.
(2) Extrinsic fault, corresponding to the insertion of an extra close-packed plane into the perfect crystal.
(3) Twin (growth) fault, located at the interface between two perfect crystallites which are in twin relation.

The stacking patterns of these faults are shown in Fig. 1 in the usual A, B, C notation.

Although the presence of intrinsic stacking faults

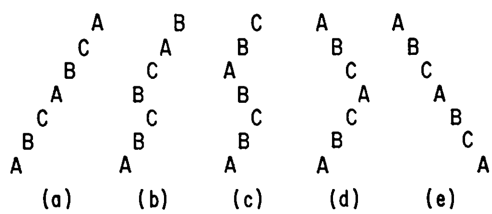

Fig. 1. Stacking sequences for: (*a*) Perfect crystal; (*b*) Intrinsic fault; (*c*) extrinsic fault; (*d*) twin fault; and (*e*) twin crystal.

in deformed face-centered cubic crystals has been verified both by X-ray diffraction (Warren & Warekois, 1955) and transmission electron microscopy methods (Howie, 1960), there is so far no direct evidence for the occurrence of extrinsic faulting in face-centered cubic crystals; however, it is possible to interpret the observed asymmetry of the shifted peaks in deformed α-brass (Wagner, 1957) as being due to a mixture of intrinsic and extrinsic faults, with intrinsic faults predominating (B. E. Warren, private communication). It is therefore worth while to set down some of the possible means of generating extrinsic faults:

(1) Condensation of a sheet of interstitials, without offset (Read, 1953).
(2) Combination of a Shockley partial dislocation with a total dislocation on a different slip plane, and subsequent dissociation into a positive Frank partial and a new Shockley partial connected by a ribbon of extrinsic stacking fault (Read, 1953).
(3) Some of the rare earths (*e.g.*, cerium) transform at low temperatures from face-centered cubic to a hexagonal lattice with *ABAC* stacking. Reference to Fig. 1(*c*) shows that an extrinsic fault produces, locally, this *ABAC* stacking. If such a material were deformed in the face-centered cubic state at a temperature somewhat above the transformation temperature it is possible that the stacking faults associated with extended dislocations would be predominantly extrinsic (H. M. Otte, private communication).

The diffraction effects produced by intrinsic faults, growth faults or a mixture of the two have been studied by several authors (Paterson, 1952; Gevers, 1954; Warren & Warekois, 1955). An extensive discussion has been given by Warren (1959). In the present work the diffraction pattern of a face-centered cubic crystal containing extrinsic faults is derived, subject to the following assumptions:

(1) Only extrinsic faults are present.
(2) Faults occur independently on only one set of parallel close-packed planes.
(3) The crystal is infinite in size (particle-size broadening neglected), and the faults cover entire (111) planes.

Formulation of the diffraction problem

In the following, the diffraction problem for faulted face-centered cubic crystals is formulated along the lines followed by Warren & Warekois (1955) in their study of intrinsic faulting. A slightly more general approach is required to allow for the more complicated structure of extrinsic faults.

The layer structure of face-centered cubic crystals may be described by noting that, for the perfect lattice, successive close-packed planes are offset laterally by a constant vector. For the stacking of (111) planes there are only two different offset vectors leading to close-packed structures (Read, 1953): $\pm\mathbf{f}=\pm(a_0/6)[1\bar{2}1]$. Faults can be described by sequences of offset vectors:

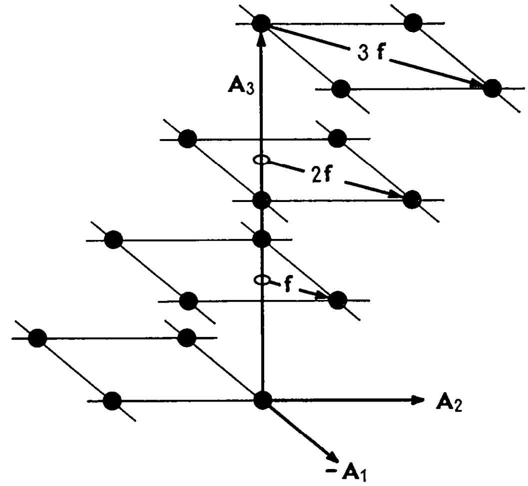

Fig. 2. Perspective view of the hexagonal lattice representation of the layer structure of a face-centered cubic crystal.

(i) Intrinsic stacking fault: $\ldots+++-+++\ldots.$
(ii) Extrinsic stacking fault: $\ldots+++--++\ldots.$
(iii) Twin fault: $\ldots++++----\ldots.$ (1)

It is convenient (Paterson, 1953) to discuss the diffraction pattern in terms of a hexagonal lattice which, with reference to the cubic unit cell of side a_0, has axes $\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3$ and reciprocal lattice vectors $\mathbf{B}_1, \mathbf{B}_2, \mathbf{B}_3$ (see Fig. 2):

$$\begin{aligned} \mathbf{A}_1&=(a_0/2)[\bar{1}10] & \mathbf{B}_1&=(2/3a_0)[\bar{2}11] \\ \mathbf{A}_2&=(a_0/2)[0\bar{1}1] & \mathbf{B}_2&=(2/3a_0)[\bar{1}\bar{1}2] \\ \mathbf{A}_3&=a_0[111] & \mathbf{B}_3&=(1/3a_0)[111]\,. \end{aligned} \quad (2)$$

$\mathbf{A}_1$ and $\mathbf{A}_2$ lie in (111) while $\mathbf{A}_3$ is normal to (111). This choice for the unit cell reflects the fact that the face-centered cubic lattice repeats at every third (111) plane ($\pm 3\mathbf{f}$ is a lattice translation vector). The relation between the indices (HKL) in the hexagonal lattice and the indices (hkl) in the cubic lattice is (Warren & Warekois, 1955)

$$\begin{aligned} H &= \tfrac{1}{2}[-h+k] \\ K &= \tfrac{1}{2}[-k+l] \\ L &= [h+k+l] \end{aligned} \quad (3)$$

In terms of the hexagonal lattice, the atoms of a (possibly faulted) face-centered cubic crystal lie at positions

$$\mathbf{r}_m=m_1\mathbf{A}_1+m_2\mathbf{A}_2+\tfrac{1}{3}m_3\mathbf{A}_3+\boldsymbol{\delta}(m_3) \quad (4)$$
$$m_1, m_2, m_3=0, \pm 1, \pm 2, \ldots$$

where $\mathbf{r}_m$ is the position of the m_1, m_2 atom in the m_3 layer. If the crystal is perfect then either

Table 1. *Phase changes for faulted face-centered cubic crystals*
(Units of $\varphi_0=(2\pi/3)$)

	$(H-K)=2 \bmod 3$	$(H-K)=1 \bmod 3$	$(H-K)=0 \bmod 3$
Normal crystal	$\ldots++++++++\ldots$	$\ldots---------\ldots$	...0000000...
Intrinsic fault	$\ldots+++-+++\ldots$	$\ldots---+---\ldots$	...0000000...
Extrinsic fault	$\ldots+++--++\ldots$	$\ldots---++--\ldots$	...0000000...
Twin fault	$\ldots++++---\ldots$	$\ldots----+++\ldots$	...0000000...
Twin crystal	$\ldots---------\ldots$	$\ldots++++++++\ldots$	...0000000...

$$\mathbf{\delta}(m_3)=m_3\mathbf{f} \tag{5}$$

or

$$\mathbf{\delta}(m_3)=-m_3\mathbf{f} \tag{6}$$

for all m_3. (The two choices correspond to 'normal' and 'twin' crystals). The presence of faults distributed at random changes equations (5), (6) into

$$\mathbf{\delta}(m_3)=q(m_3)\mathbf{f} \tag{7}$$

where $q(m_3)$ is a stochastic variable* taking on positive and negative integral values.

Having specified the nature of the atomic displacements introduced by faulting on (111), we can now proceed to an expression for the diffracted intensity which explicitly contains the effects produced by faulting.

If a beam of X-rays of wavelength λ directed along $\mathbf{s}_0$ traverses an infinite crystal containing atoms at positions $\mathbf{r}_m$, then (Warren, 1959)

$$I(\mathbf{s}-\mathbf{s}_0) = C\sum_m\sum_n \exp\{(2\pi i/\lambda)(\mathbf{s}-\mathbf{s}_0).(\mathbf{r}_m-\mathbf{r}_n)\} \tag{8}$$

is the intensity diffracted into the direction $\mathbf{s}$; here C depends upon the scattering power of the atoms. On defining components h_1, h_2, h_3 in reciprocal space through

$$(1/\lambda)(\mathbf{s}-\mathbf{s}_0)=h_1\mathbf{B}_1+h_2\mathbf{B}_2+h_3\mathbf{B}_3\,, \tag{9}$$

noting that $\mathbf{A}_i.\mathbf{B}_j=\delta_{ij}$ and $\mathbf{\delta}(m_3).\mathbf{B}_3=0$, equation (8) becomes

$$I(h_1, h_2, h_3) = C\sum_m\sum_n \exp\{2\pi i[(m_1-n_1)h_1+(m_2-n_2)h_2 + \tfrac{1}{3}(m_3-n_3)h_3]\}.\exp\{2\pi i[h_1\mathbf{B}_1+h_2\mathbf{B}_2].[\mathbf{\delta}(m_3)-\mathbf{\delta}(n_3)\}. \tag{10}$$

The summations over m_1, n_1, m_2, n_2 can be carried out immediately, yielding

$$I(h_1, h_2, h_3) = C\delta(h_1-H)\delta(h_2-K)\sum_{m_3=-\infty}^{\infty}\sum_{n_3=-\infty}^{\infty} \times\exp\{(2\pi i h_3/3)(m_3-n_3)\} \times\exp\{2\pi i[H\mathbf{B}_1+K\mathbf{B}_2].[\mathbf{\delta}(m_3)-\mathbf{\delta}(n_3)]\}\,, \tag{11}$$

where H, K are integers and $\delta(X)$ is the Dirac delta function. The diffracted intensity vanishes except when $h_1=H$ and $h_2=K$, independent of the presence of faults. Bearing this in mind, the diffracted intensity can be written (in arbitrary units) as

$$I(h_3) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\exp\{(2\pi i h_3/3)(m-n)\} \times\exp\{2\pi i[H\mathbf{B}_1+K\mathbf{B}_2].[\mathbf{\delta}(m)-\mathbf{\delta}(n)]\}\,. \tag{12}$$

The argument of the second exponential in equation (12) is the phase difference Φ_{mn} between X-rays scattered through $H\mathbf{B}_1+K\mathbf{B}_2$ by the m and by the n layers. Since, in the presence of faulting, $\mathbf{\delta}(m)$ is a stochastic variable, Φ_{mn} is a stochastic variable as well: in equation (12), $\exp\{i\Phi_{mn}\}$ must be replaced by its expectation value over the distribution of Φ_{mn}. Thus

$$I(h_3) = \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\exp\{(2\pi i h_3/3)(m-n)\}\langle\exp\{i\Phi_{mn}\}\rangle\,. \tag{13}$$

Equation (13), together with information about the phase shifts Φ_{mn} introduced by faults, contains all the diffraction effects which are produced by faulting in the present model.

For a given reflection H, K the value of Φ_{mn} is readily found. If a 'normal' crystal is defined by the (constant) stacking offset vector $+\mathbf{f}$, then for a perfect crystal

$$\begin{aligned}\Phi_{mn}&=+(m-n)(2\pi/3) &&\text{for } (H-K)=2 \bmod 3\\ \Phi_{mn}&=-(m-n)(2\pi/3) &&\text{for } (H-K)=1 \bmod 3\\ \Phi_{mn}&=+(m-n)2\pi &&\text{for } (H-K)=0 \bmod 3\,.\end{aligned} \tag{14}$$

Defining, for convenience, $\varphi_0=(2\pi/3)$, the sequence of phase changes across successive planes can be tabulated for faulted as well as perfect crystals; with

$$\Phi_{mn} = \sum_{k=m+1}^{n}\varphi_k\,,$$

the φ_k are given in Table 1, from which it is clear that reflections $H-K=0 \bmod 3$ are not affected by faults.

The expectation value $\langle\exp\{i\Phi_{mn}\}\rangle$ can be found by considering an appropriate random walk in the individual phase changes φ_i.*

Since the calculation for intrinsic faulting is parallel to that for extrinsic faulting while being considerably less complicated, and since it is desirable to reproduce the results for intrinsic faulting for purposes of comparison, the intrinsic faulting case will be treated briefly before proceeding to a consideration of extrinsic faulting.

* Note that relationships may exist among $q(m_3)$ and $q(m_3+k)$, $k=0, \pm1, \pm2, \ldots$, due to the structure of the faults.

* For intrinsic faults it is scarcely necessary to use the random walk machinery: the expectation value can be written down immediately.

Diffraction by a crystal containing intrinsic faults

Let the crystal contain intrinsic faults with stacking fault probability α. We treat the case $(H-K)=2 \bmod 3$. (The case $(H-K)=1 \bmod 3$ is found by changing φ_0 to $-2\pi/3$, while for $(H-K)=0 \bmod 3$ the diffracted intensity pattern is not affected by faulting).

Defining $N=m-n$ and $\xi=2\pi h_3/3$, equation (13) can be written

$$I(\xi,\alpha) = \sum_{m=-\infty}^{\infty}\left[\sum_{N=-\infty}^{\infty}[\exp[iN\xi]]\,\langle\exp i\Phi_N\rangle\right] \quad (15)$$

where

$$\Phi_0 = 0\,,$$
$$\Phi_N = \varphi_1+\varphi_2+\ldots+\varphi_N,\quad N>0\,,$$

and

$$\varphi_{(-k)} = -\varphi_k\,. \quad (16)$$

The individual phase shifts φ_i between successive (111) planes take the values $+\varphi_0$ and $-\varphi_0$ with probabilities $(1-\alpha)$ and α, respectively.

The probability of finding a given phase difference $\Phi_N=q(N)\varphi_0$ is therefore the same as the probability $p(q, N)$ of finding a displacement $q(N)$ after a (one-dimensional) random walk of N steps of unit length in which negative steps occur with probability α.

Now

$$p(q=N-2k, N) = \frac{N!}{k!(N-k)!}\,\alpha^k(1-\alpha)^{N-k}$$

so that

$$P(N-2k, N) = \frac{N!}{k!(N-k)!}\,\alpha^k(1-\alpha)^{N-k} \quad (17)$$

is the probability of finding a phase difference $\Phi_N=(N-2k)\varphi_0$. Therefore, since

$$\langle\exp i\Phi_N\rangle = \sum_{k=0}^{N}P(N-2k, N)\times\exp i(N-2k)\varphi_0,\quad (N\geq 0),$$

$$\langle\exp i\Phi_N\rangle = \sum_{k=0}^{N}\frac{N!}{k!(N-k)!}\times(\alpha\exp-i\varphi_0)^k[(1-\alpha)\exp i\varphi_0]^{N-k},\quad (N\geq 0)\,,$$

which can be summed using the binomial theorem:

$$\langle\exp i\Phi_N\rangle=[\alpha\exp[-i\varphi_0]+(1-\alpha)\exp[i\varphi_0]]^N,\quad (N\geq 0)\,. \quad (18)$$

From equations (16) it is clear that, for $N<0$, the roles of $+\varphi_0$ and $-\varphi_0$ are simply interchanged:

$$\langle\exp i\Phi_N\rangle=[\alpha\exp[i\varphi_0]+(1-\alpha)\exp[-i\varphi_0]]^{|N|},\quad N<0\,. \quad (19)$$

On substituting equations (18) and (19) into equation (15)

$$I(\xi,\alpha) = \sum_{m=-\infty}^{\infty}[1+\{\sum_{N=1}^{\infty}\exp[iN\xi][\alpha\exp[-i\varphi_0] + (1-\alpha)\exp[i\varphi_0]]^N+\text{c.c.}\}]\,. \quad (20)$$

Since all lattice planes are statistically equivalent, the summation over m is trivial, yielding only a (suppressed) normalization factor. On defining

$$z=[\alpha\exp[i(\xi-\varphi_0)]+(1-\alpha)\exp[i(\xi+\varphi_0)]]\,,$$

equation (20) can be written

$$I(\xi,\alpha)=\{1+\sum_{N=1}^{\infty}[z^N+(z^*)^N]\}=1+\frac{z}{1-z}+\frac{z^*}{1-z^*}\,,$$

valid for $|z|<1$. The condition $|z|<1$ is satisfied for $0<\alpha<1$, $\varphi_0\neq 0$, so that

$$I(\xi,\alpha) = 1+\left\{\frac{\alpha\exp[i(\xi-\varphi_0)]+(1-\alpha)\exp[i(\xi+\varphi_0)]}{1-(1-\alpha)\exp[i(\xi+\varphi_0)]-\alpha\exp[i(\xi-\varphi_0)]}+\text{c.c.}\right\},\quad 0<\alpha<1\,. \quad (21)$$

Upon carrying out the indicated algebra and setting $\varphi_0=(+2\pi/3)$ (corresponding to $H-K=2 \bmod 3$),

$$I(\xi,\alpha)=3\alpha(1-\alpha)[(2-3\alpha+3\alpha^2)+\cos\xi + \sqrt{(3)}(1-2\alpha)\sin\xi]^{-1},\quad (H-K)=2 \bmod 3\,, \quad (22)$$

which is identical with the result given by Paterson (1952). Equation (22) represents a peak with maximum at

$$\xi_{\max}=\tan^{-1}\sqrt{(3)}(1-2\alpha)\,,$$

symmetric about $\xi_{\max}$. Further symmetry properties of $I(\xi,\alpha)$ are readily seen from equation (21):

$$I(\xi,\alpha)=I(-\xi,1-\alpha)$$

and the relation between reflections $(H-K)=2 \bmod 3$ and $(H-K)=1 \bmod 3$

$$(H-K)=2 \bmod 3 \qquad (H-K)=1 \bmod 3$$
$$I_2(\xi,\alpha)=I_1(-\xi,\alpha)$$
$$I_2(\xi,\alpha)=I_1(\xi,1-\alpha)\,.$$

For purposes of comparison with the results of the

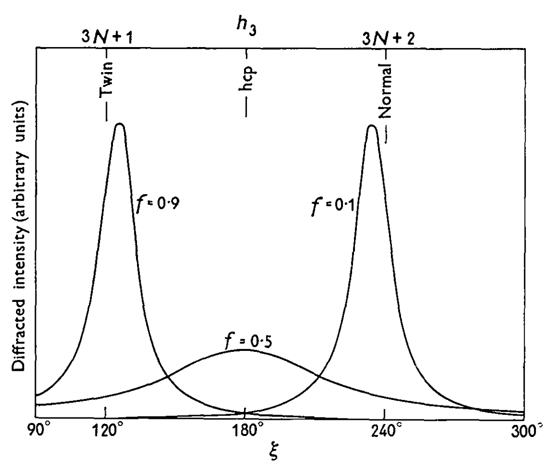

Fig. 3. Diffracted intensity as a function of h_3 (see text) for various degrees of intrinsic faulting.

extrinsic fault calculation it is convenient to specify the degree of faulting by f, the fraction of (111) planes faulted. For intrinsic faulting f is identical with the stacking fault probability α.

The intensity $I(\xi,\alpha)\equiv I(\xi,f)$ is plotted against ξ or h_3 (recall $\xi=2\pi h_3/3$) for $f=0{\cdot}1$, $0{\cdot}5$, $0{\cdot}9$ in Fig. 3. The displacement of the intensity maximum, $\xi_{\max}$, with increasing f is shown in Fig. 5, where it is contrasted with the behavior of the diffraction maxima shown by a crystal containing extrinsic faults.

Diffraction by a crystal containing extrinsic faults

As in the case of intrinsic faulting, the expectation value $\langle\exp i\Phi_{mn}\rangle$ can be found by considering a random walk process. Reference to Table 1 shows that the phase differences between successive (111) layers are no longer independent: negative phase differences, produced by faulting, must occur in pairs. Therefore, the appropriate random walk to consider is one in which the possible steps are $+1$ (occurring with probability $1-\beta$) and -2 (probability β). Let the probability of finding a displacement $q(L)$ after L steps be $p(q,L)$:

$$p(q=L-3k,\,L)=\frac{L!}{k!\,(L-k)!}\,\beta^k(1-\beta)^{L-k}\,. \tag{23}$$

It is now necessary to relate the possible sequences $n\to m$ of (111) lattice planes to this random walk.

Consider a large crystal made up of M close-packed planes and containing r extrinsic faults. The number of random steps made in traversing the crystal is $M-r$, of which r steps have the value -2. Thus $\beta=r/(M-r)$.

In considering all the possible lattice plane sequences $n\to m$ in such a crystal, account must be taken of the fact that r of the lattice planes (those 'halfway through' an extrinsic fault) cannot be represented directly as either the beginning or the end of a random walk: lattice plane sequences $n\to m$ beginning or ending with these *extraordinary* planes must be treated separately.

Suppose we have a lattice plane sequence $n\to m$ in which both n and m are *ordinary* planes. The corresponding random walk is readily found: a random walk of L steps, of which k are negative, corresponds to $m-n=L+k$ lattice planes and to a phase difference $\Phi_{mn}=(L-3k)\varphi_0$ across them. Letting $N=m-n$ be the separation of the nth and mth planes, the probability of finding a phase difference $\Phi_N=(N-4k)\varphi_0$ across them is therefore found by replacing L by $N-k$ in equation (23):

$$P(N-4k,\,N)=\frac{(N-k)!}{k!\,(N-2k)!}\,\beta^k(1-\beta)^{N-2k},\quad 0\le k\le[\tfrac12 N]$$

where the requirements that the nth (beginning) plane be ordinary and that there be a total phase difference of $(m-n-4k)\varphi_0$ ensure that the mth plane will also be ordinary. The probability that an arbitrary sequence $n\to m$ begins and ends with ordinary planes and gives a phase difference $(N-4k)\varphi_0$ is therefore obtained by multiplying the above probability by $(1+\beta)^{-1}$, the probability that the beginning plane be ordinary:

$$P_{00}[(N-4k)\varphi_0,\,N]=\left(\frac{1}{1+\beta}\right)\frac{(N-k)!}{k!\,(N-2k)!}\,\beta^k(1-\beta)^{N-2k},$$
$$0\le k\le[\tfrac12 N]\,. \tag{24}$$

The remaining three cases, in which either or both of the planes n, m are extraordinary, can be treated by simply adding an extraordinary plane (occurring with probability β) to either or both ends of an ordinary–ordinary sequence, and changing the value of the phase difference accordingly. Thus:

$$\begin{aligned}
&P_{0e}[(N-2-4k)\varphi_0,N]\\
&=P_{00}[(N-1-4k)\varphi_0,N-1].\beta, && 0\le k\le[(N-1)/2]\\
&P_{e0}[(N-2-4k)\varphi_0,N]\\
&=\beta.P_{00}[(N-1-4k)\varphi_0,N-1], && 0\le k\le[(N-1)/2]\\
&P_{ee}[(N-4-4k)\varphi_0,N]\\
&=\beta.P_{00}[(N-2-4k)\varphi_0,N-2].\beta, && 0\le k\le[(N-2)/2]\,.
\end{aligned} \tag{25}$$

Noting that equations (24), (25) incorporate the relative frequencies of occurrence of the four possible types of sequence $m\to n$, the expectation value can be written

$$\langle\exp i\Phi_{mn}\rangle\equiv\langle\exp i\Phi_N\rangle=\Sigma\{P_{00}(\Phi_N)+P_{0e}(\Phi_N)+P_{e0}(\Phi_N)+P_{ee}(\Phi_N)\}\exp i\Phi_N \tag{26}$$

where the sum is to be taken over all allowed values of Φ_N. Equation (26) has been derived for $N\ge 0$; as in the case of intrinsic faulting, the expectation value for $N<0$ is found by replacing $+\varphi_0$ by $-\varphi_0$, which is equivalent to the operation of complex conjugation:

$$\langle\exp i\Phi_N\rangle_{N<0}=[\langle\exp i\Phi_N\rangle_{N>0}]^\dagger\,. \tag{27}$$

The summation of equation (26) can be carried out in closed form since (*Higher Transcendental Functions*, 1953)

$$\sum_{k=0}^{[M/2]}\frac{(-1)^k(M-k)!}{k!\,(M-2k)!}\,(2X)^{M-2k}=U_M(X)\,, \tag{28}$$

where $U_M(X)$ is the Tchebichef polynomial of the second kind of degree M. On defining

$$X=i(1-\beta)\exp[2i\varphi_0]/(2\sqrt{\beta}) \tag{29}$$

each of the terms of equation (26) can be put in the form of equation (28), so that (26) becomes

$$\begin{aligned}
\langle\exp i\Phi_N\rangle=\frac{1}{1+\beta}\{&(-i\sqrt{\beta}\exp[-i\varphi_0])^N U_N(X)\\
&+2\beta\exp[-i\varphi_0](-i\sqrt{\beta}\exp[-i\varphi_0])^{N-1}U_{N-1}(X)\\
&+\beta^2\exp[-2i\varphi_0](-i\sqrt{\beta}\exp[-i\varphi_0])^{N-2}U_{N-2}(X)\},\\
&N\ge 0\,,
\end{aligned} \tag{30}$$

where only terms in $U_K(X)$ for which $K \geq 0$ are included.*

Recalling equation (13), and again defining $\xi = 2\pi h_3/3$, the diffracted intensity can be written

$$I(\xi, \beta) = \sum_{n=-\infty}^{\infty} \sum_{N=-\infty}^{\infty} \exp [iN\xi]\langle \exp i\Phi_N \rangle$$
$$= A \sum_{N=-\infty}^{\infty} \exp [iN\xi]\langle \exp i\Phi_N \rangle . \quad (31)$$

Since $\langle \exp i\Phi_N \rangle$ has been calculated for the average origin plane n, the constant A bears no information and is therefore dropped. Recalling equation (27), defining

$$Z = -i\sqrt{\beta} \exp [i(\xi-\varphi_0)] \quad (32)$$

and substituting for $\langle \exp i\Phi_N \rangle$, ($N \geq 0$), from equation (30)

$$I(\xi, \beta) = \langle \exp i\Phi_0 \rangle + \frac{1}{1+\beta}\left\{\sum_{N=1}^{\infty} [Z^N U_N(X) + 2\beta \times \exp [i(\xi-\varphi_0)]Z^{N-1}U_{N-1}(X) + \beta^2 \times \exp [2i(\xi-\varphi_0)]Z^{N-2}U_{N-2}(X)] + \sum_{N=1}^{\infty} [\text{c.c.}]\right\}, \quad (33)$$

where, again, only the terms in $U_K(X)$ for which $K \geq 0$ are to be included.

The summations of equation (33) can now be carried out with the help of the generating function for $U_N(X)$ (*Higher Transcendental Functions*, 1953):

$$1/(1-2XZ+Z^2) = \sum_{N=0}^{\infty} U_N(X)Z^N, \quad |Z^2-2XZ| < 1 . \quad (34)$$

The condition $|Z^2-2XZ|<1$ is met provided that $0<\beta<1$ and $\varphi_0 \neq 0$. Noting that $\langle \exp i\Phi_0 \rangle = 1$ and employing equation (34), equation (30) becomes

The diffracted intensity $I_-(\xi, \beta)$, corresponding to $H-K=1$ mod 3, is obtained by replacing ξ by $(-\xi)$ in equation (37); when $H-K=0$ mod 3 the diffracted intensity is, as noted before, unaffected by faulting.

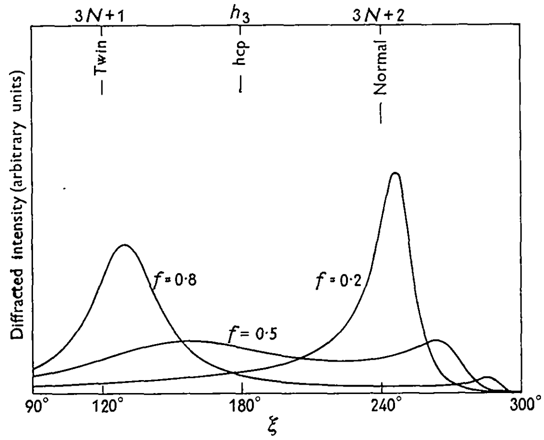

Fig. 4. Diffracted intensity as a function of h_3 (see text) for various degrees of extrinsic faulting.

Equations (22) and (37) give the diffracted intensity for face-centered cubic crystals containing intrinsic and extrinsic faults, respectively. While some analytic results for low extrinsic fault density are given in the next section, the properties of equation (37) for general values of β are, unfortunately, not easily specified analytically; the information is most readily presented by means of diffracted intensity profiles, as in Fig. 4, and by a plot of the positions of the maxima in the diffracted intensity profiles versus f,

$$I(\xi, \beta) = 1 + \frac{1}{1+\beta}\left\{\frac{2XZ-Z^2+2\beta \exp [i(\xi-\varphi_0)] + \beta^2 \exp [2i(\xi-\varphi_0)]}{1-2XZ+Z^2} + \text{c.c.}\right\}$$

or, on replacing X and Z by their values,

$$I(\xi, \beta) = 1 + \frac{1}{1+\beta}\left\{\frac{(1-\beta) \exp [i(\xi+\varphi_0)] + \beta(1+\beta) \exp [2i(\xi-\varphi_0)] + 2\beta \exp [i(\xi-\varphi_0)]}{1-(1-\beta) \exp [i(\xi+\varphi_0)] - \beta \exp [2i(\xi-\varphi_0)]} + \text{c.c.}\right\},$$
$$0<\beta<1, \quad \varphi_0 \neq 0 . \quad (35)$$

Upon carrying out the indicated algebra, equation (35) becomes

$$I(\xi, \beta) = \frac{\beta(1-\beta)}{(1+\beta)}\left\{\frac{2-\cos (\xi+\varphi_0) + 2 \cos (\xi-\varphi_0) - 2 \cos 2\varphi_0 - \cos (\xi-3\varphi_0)}{(1-\beta+\beta^2)-(1-\beta) \cos (\xi+\varphi_0) - \beta \cos 2(\xi-\varphi_0) + \beta(1-\beta) \cos (\xi-3\varphi_0)}\right\}$$
$$0<\beta<1, \quad \varphi_0 \neq 0 . \quad (36)$$

Specializing to the case $\varphi_0 = +2\pi/3$ (corresponding to $(H-K)=2$ mod 3),

$$I_+(\xi, \beta) = \frac{3\beta(1-\beta)}{(1+\beta)}\left\{\frac{2-\cos \xi + \sqrt{3} \sin \xi}{2(1-\beta+\beta^2)+(1+\beta-2\beta^2) \cos \xi + \sqrt{(3)}(1-\beta) \sin \xi + \beta \cos 2\xi + \sqrt{(3)}\beta \sin 2\xi}\right\}$$
$$0<\beta<1, \quad (H-K)=2 \text{ mod } 3, \quad \xi=2\pi h_3/3 . \quad (37)$$

the fraction of (111) planes faulted, as in Fig. 5. (For intrinsic faulting f, the fraction of planes faulted is just α, while for extrinsic faulting it is $2\beta/(1+\beta)$.)

From Figs. 4 and 5, the characteristics of $I(\xi, \beta)$

* The recurrence relation

$$U_{N-1}(X) = 2XU_N(X) - U_{N+1}(X)$$

can be used to show, by finite induction, that the probabilities of equation (26) sum to 1 for all N.

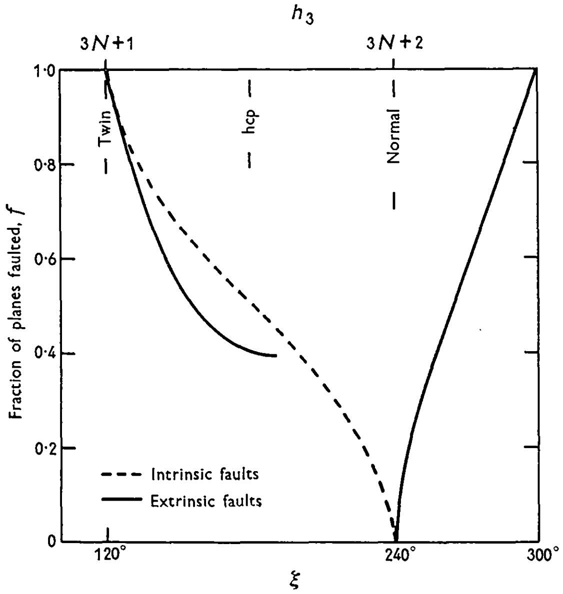

Fig. 5. Peak positions in reciprocal space as a function of degree of faulting for intrinsic and extrinsic faults.

for extrinsic faulting are (as f, the degree of faulting, increases from 0):

(1) A shift in the peak position directed away from the 'twin' reflection position and accompanied by an asymmetric broadening, the shift increasing monotonically as the degree of faulting increases.
(2) The appearance, when roughly 40% of the lattice planes are faulted, of a new peak, also asymmetric, near the hexagonal close-packed lattice reflection position.
(3) The simultaneous growth and shift toward the twin position of this new peak, coupled with a continued shrinkage of the original peak, until, as $\beta \to 1$, a sharp peak is formed at the twin position.
(4) The gross effect is that for intermediate degrees of faulting, the diffraction pattern is streaked along the h_3 direction, with the streaking extending further toward the twin position (decreasing h_3) than along increasing h_3.

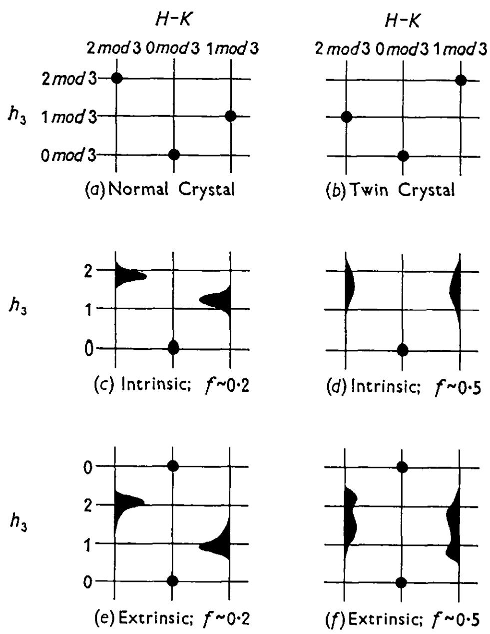

Fig. 6. Reciprocal space intensity maps for faulted crystals.

The changes in diffracted intensity produced by intrinsic and extrinsic faults are contrasted in Fig. 6, where, following Paterson (1952), schematic maps of the intensity distribution in the hexagonal reciprocal lattice are shown for various types and degrees of faulting.

Fourier series expansion

From equation (31) it is clear that a Fourier expansion of the diffracted intensity about $\xi=0$ is

$$I(\xi,\beta)=\sum_{n=-\infty}^{\infty} A_N(\beta)\exp iN\xi \tag{38}$$

with

$$A_N(\beta)=\langle \exp i\Phi_N\rangle\,.$$

As Warren (1959) has emphasized, greater interest attaches to a Fourier series expansion about the peak position $\xi_{\max}$. For extrinsic faulting this is only possible when $f \lesssim 0·4$, since at greater degrees of faulting two peaks occur. However, provided $f \lesssim 0·4 (\beta \lesssim 0·25)$, a formal expansion about $\xi_{\max}$ is readily given. It is only necessary to write (38) as

$$I(\xi-\xi_{\max},\beta)=\sum_{N=-\infty}^{\infty}\exp\left[iN(\xi-\xi_{\max})\right]A'_N(\beta) \tag{39}$$

with

$$A'_N(\beta)=\exp\left[iN\xi_{\max}\right]\langle \exp i\Phi_N\rangle$$

or, in real form,

$$I(\xi-\xi_{\max},\beta)=1+\sum_{N=1}^{\infty}\{a_N\cos N(\xi-\xi_{\max}) + b_N \sin N(\xi-\xi_{\max})\}$$

with

$$a_N=\exp\left[iN\xi_{\max}\right]\langle \exp i\Phi_N\rangle + \exp\left[-iN\xi_{\max}\right]\langle \exp i\Phi_N\rangle^{\dagger}$$

$$b_N=i\left[\exp\left[iN\xi_{\max}\right]\langle \exp i\Phi_N\rangle - \exp\left[-iN\xi_{\max}\right]\langle \exp i\Phi_N\rangle^{\dagger}\right]. \tag{40}$$

Diffraction effects at low extrinsic fault densities

When $f=0$ (*i.e.*, the crystal is perfect) an infinitely sharp peak in $I_+(\xi,\beta)$ occurs at $\xi=4\pi/3$. To examine the behavior of $I_+(\xi,\beta)$ for small β (small f), equation (37) is therefore written in terms of the new angle $\delta=\xi-(4\pi/3)$; an expansion is then obtained by assuming that both β and δ are small. On substituting

$$\xi=\delta+(4\pi/3)$$

in equation (37) we obtain

$$I_+(\delta, \beta) = \frac{3\beta(1-\beta)}{(1+\beta)} \left\{ \frac{2-\cos\delta - \sqrt{3}\sin\delta}{2(1-\beta+\beta^2)+(\beta^2+\beta-2)\cos\delta + \sqrt{(3)}\beta(1-\beta)\sin\delta + \beta\cos 2\delta - \sqrt{(3)}\beta\sin 2\delta} \right\} \quad (41)$$

which gives, to second order in δ and β,

$$I_+(\delta, \beta) \simeq \frac{3\beta(1-\sqrt{(3)}\delta)}{3\beta^2 - \sqrt{(3)}\beta\delta + \delta^2} + 0(\delta^3, \delta^2\beta, \ldots)\,. \quad (42)$$

Equation (42) shows a peak at

$$\delta_{\max} \simeq \frac{\sqrt{3}}{2}\beta$$

of height

$$I_{+\max} \simeq \frac{4}{3\beta}$$

and with half-width limits δ_1, δ_2 given by

$$\delta_1 \cong \frac{\sqrt{3}}{2}\beta - \frac{3}{2}\beta$$

$$\delta_2 \cong \frac{\sqrt{3}}{2}\beta + \frac{3}{2}\beta$$

so that the width at half-maximum intensity is, to this order of approximation, 3β. (Note that to this approximation the broadening is symmetric).

These parameters may be compared directly with the corresponding parameters for intrinsic faulting when the density of faulting is specified by f, the fraction of planes faulted. This is done in Table 2.

Table 2. *Diffraction effects at low fault densities ($f \ll 1$) for reflections $(H-K)=2$ mod 3*

Parameter	Intrinsic faulting*	Extrinsic faulting
Peak shift, $\delta_{\max}$	$-(\sqrt{3})/(2)f$	$+(\sqrt{3})/(4)f$
Peak intensity, $I_{+\max}$	$4/(3f)$	$8/(3f)$
Half-width	$3f$	$(3/2)f$

* Some of these values have been given by Paterson (1952) and by Warren & Warekois (1955).

Summary

The diffraction effects produced by extrinsic faulting are qualitatively different from the effects produced by intrinsic faulting, and should be experimentally distinguishable.

The calculation has been carried out under the assumption that only extrinsic faults are present, and gives no direct information about the case in which a mixture of extrinsic and intrinsic faults occur in the same crystal. One remark can, however, be made. The line broadening duc to intrinsic faulting is symmetric, while that due to extrinsic faulting is not. Therefore, it is clear that the addition of extrinsic faults to a crystal originally containing only intrinsic faults will always destroy the symmetry of the broadened lines.

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