Acta Cryst. (1957). **10**, 447

X-ray Diffraction from Body-Centred Cubic Crystals Containing Stacking Faults

By P. B. Hirsch

Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England

and H. M. Otte

Department of Physical Metallurgy, University of Birmingham, England

(*Received* 3 *December* 1956 *and in revised form* 14 *February* 1957)

This paper presents calculations of the intensities diffracted from polycrystalline specimens of body-centred cubic crystals containing stacking faults on (211) planes. Possible applications of the theory to the anomalous line broadening from martensite and from cold-worked iron are discussed.

Introduction

The possibility of errors in the stacking of the (112) planes in b.-c.c. metals has received only cursory attention (Barrett, 1949; Cottrell & Bilby, 1951; Cottrell, 1953; Frank & Nicholas, 1953; Suzuki, 1954), mainly because direct experimental evidence of their existence is lacking. The importance of stacking errors (or faults) in f.-c.c. structures, however, is well established and studies have been made of faulting induced by deformation (Warren & Warekois, 1955; Barrett, 1952; Hirsch, Kelly & Menter, 1955) as well as during phase transformations (Barrett, 1950, 1952). Faults in b.-c.c. structures may be more difficult to detect and to identify because their occurrence may be less frequent, since the energy involved in the formation of a b.-c.c. twin is much greater than in those f.-c.c. metals which twin and fault easily (Cahn, 1954).

The importance of faulting in the cold working of b.-c.c. metals has not been established, but in view of a recent theory (Wechsler, Lieberman & Read, 1953) of the crystallographic aspects of the martensite transformation it seems worth while to consider whether faulting could be a possible contributing factor to the exceptional broadening of Debye–Scherrer rings from martensite in steels (Wheeler & Jaswon, 1947; Smith, 1953). According to this theory, the martensite plate could be either a single crystal in which approximately every sixth (112) plane has slipped one interatomic distance in the $[11\bar{1}]$ direction, or a twinned crystal in which the ratio of the thickness of the twin lamellae is approximately 2:1, and in which the twinning plane is (112). In either case the calculation yields the same result for the habit plane and orientation relationship between the austenite and the martensite. Consequently, the martensite could, according to the theory, contain an arbitrary amount of twins without in essence affecting the results of the theory. Such twins, if only one atomic layer thick, would, in fact, be stacking faults. Further, if the transformation proceeds by the movement of partial dislocations with Burgers vectors $[11\bar{1}]/6$ lying in (112) planes (Cottrell, 1953), such twins and stacking faults would be expected to occur. In the diffusionless ('martensitic') phase transformations of Co (f.-c.c. → h.c.p.) (Edwards & Lipson, 1942), Li and Na(b.-c.c. → h.c.p. or f.-c.c.) (Barrett, 1950, 1956), for example, the product phase is faulted.

Stacking faults may also possibly be of importance in the deformation of b.-c.c. crystals; thus it is known that twins can be produced by deformation in Fe (Kelly, 1953; Paxton, 1953). The broadening of the X-ray lines from Fe filings (Smallman, 1953) shows certain anomalies similar to those found for martensite. The purpose of the present paper is to examine the X-ray diffraction effects from faults in b.-c.c. structures and to discuss a possible interpretation of the results on line broadening from martensite and iron.

The nature of stacking faults in b.-c.c crystals

In the f.-c.c. case two types of fault may be distinguished: (i) A growth fault, which forms the boundary between two twins, e.g.

$$\ldots A\,B\,C\,A\,B\,\underline{A}\,C\,B\,A\,C\,B\,A \ldots .$$

(ii) A deformation fault in which the packing sequence is always the same except at a fault plane:

$$\ldots A\,B\,C\,A\,B\,\underline{A}\,B\,C\,A\,B\,C \ldots .$$

This is actually equivalent to two adjacent growth faults. The fault occurs on a (111) plane, which is the twinning plane and also the most densely packed plane. In the b.-c.c. case, the twinning plane is (112) and is the only plane on which faulting could occur, even though (110) is the most densely packed plane (Barrett, 1949).

The stacking sequence of (112) planes in b.-c.c. crystals may be described as

$$\ldots A_1A_2B_1B_2C_1C_2A_1A_2B_1B_2 \ldots .$$

Successive layers are displaced relative to each other by a vector with components $[11\bar{1}]/6$ and $[1\bar{1}0]/2$

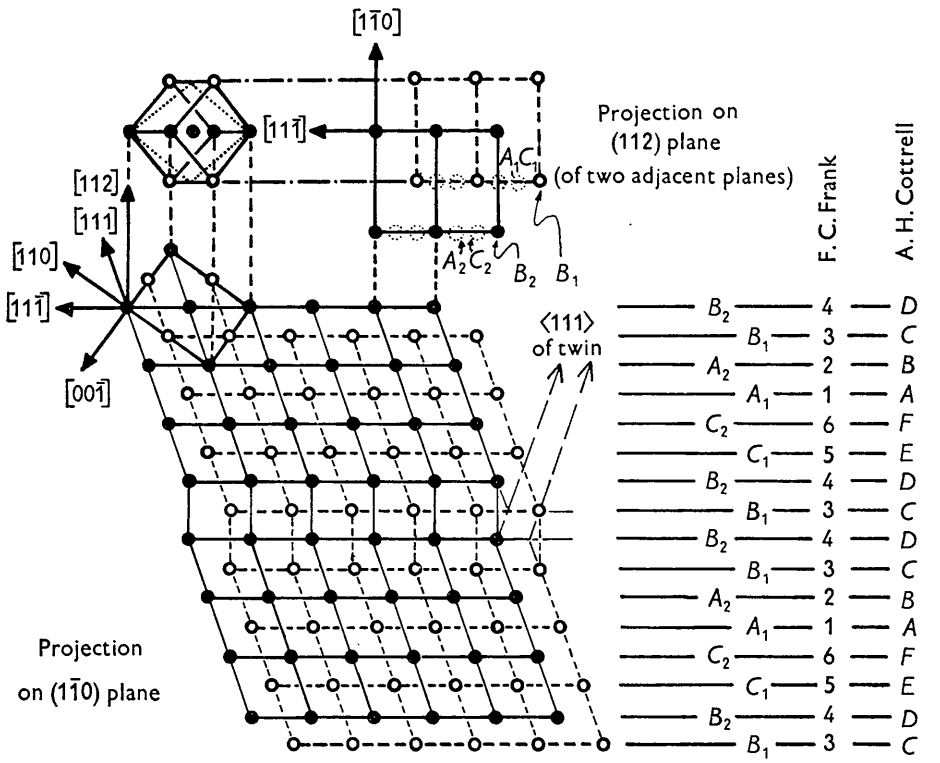

Fig. 1. Projection of the b.-c.c. structure on a {112} and a {110} plane; the latter projection shows the effect of an error in the stacking sequence of the (112) planes.

along the [11$\bar{1}$] and [1$\bar{1}$0] axes respectively (Fig. 1). A sequence of six layers defines the stacking arrangement completely. A fault occurs when, for example, B_2, instead of being followed by C_1, is followed by B_1 again. The displacement of B_1 relative to B_2 has components $-[11\bar{1}]/3$ and [1$\bar{1}$0] along the axes, and since displacements [1$\bar{1}$0] cannot be distinguished inside the crystal the fault is effectively produced by a displacement $-[11\bar{1}]/3$, which is also equivalent to a displacement $[11\bar{1}]/6$, in the [11$\bar{1}$] direction (Fig. 1). Faults are therefore produced by wrong displacements in the [11$\bar{1}$] directions only.

A growth fault in b.-c.c. crystals can occur in the same way as in f.-c.c.* crystals; it gives rise to the sequence

$$\ldots B_1B_2C_1C_2A_1A_2B_1B_2\underline{B_1}A_2A_1C_2C_1B_2\ldots$$

and produces a twin orientation.

A deformation fault is produced analogously thus:

$$\ldots B_1B_2C_1C_2A_1A_2B_1B_2\underline{B_1}B_2C_1C_2A_1A_2B_1\ldots$$

and is illustrated in Fig. 1. This fault preserves neither nearest-neighbour distances nor the correct bond angles (though the distances between neighbouring planes are preserved). It is therefore difficult to consider this kind of fault as a twin of minimum thickness and thus the analogy with the f.-c.c. case breaks down here. However, if a fault occurs at every layer the twin orientation is produced.

Effect of stacking faults on X-ray reflexions

In the b.-c.c. case stacking faults are produced by wrong components of displacement in the [11$\bar{1}$] directions. In the unfaulted crystal successive (112) planes are displaced relative to each other by a vector with a component $[11\bar{1}]/6$ in the [11$\bar{1}$] direction. Since each layer has equivalent atomic positions at 0 and $[11\bar{1}]/2$, a sequence of only three layers (with positions at 0, $[11\bar{1}]/6$, $[11\bar{1}]/3$) is needed to describe the pattern of displacements along the [11$\bar{1}$] direction completely (see Fig. 1). Therefore, if only the position of the layers along the [11$\bar{1}$] axis is considered, the sequence can be described simply as

$$A\ B\ C\ A\ B\ C\ \ldots \text{ etc.},$$

i.e. as a sequence of three layers rather than as a sequence of six layers necessary when the position of the layers along the [1$\bar{1}$0] direction is also taken into account. The calculation for the probability of finding a layer in any of the three positions along the [11$\bar{1}$] axis reduces therefore to that relevant to the f.-c.c. case (Paterson, 1952; Warren & Warekois, 1955), and the results obtained for the latter case can be adapted

* It should be noted that the definition is not exactly the same as in the f.-c.c. case, since a complete sequence consists of 6 layers instead of only 3.

easily for b.-c.c. structures. The calculations have been carried out for random distributions of deformation faults and of growth faults. It should be noted that if the martensite transformation takes place by the movement of partial dislocations (Cottrell, 1953) the resulting distributions of faults may not conform to either of these random distributions. Thus, if the partial dislocations merely separate, deformation faults are produced; if they rotate about single dislocations with screw components [112]/6, twins are produced whose thickness depends on the number of revolutions; rotation about several dislocations with screw components [112]/6 would result in the formation of more complex arrangements of faults. Thus the final martensite plate might be expected to contain both deformation and growth faults.

(1) *Transformation of axes*

For the calculation of X-ray intensities it is convenient to choose orthorhombic coordinates as follows. Let $\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3$ be the b.-c.c. axes and *hkl* the corresponding indices. In terms of one set of (112) planes, introduce a new set of orthogonal axes $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ with $\mathbf{a}_1, \mathbf{a}_2$ in the (112) plane and $\mathbf{a}_3$ normal to it. Let *HKL* be the new indices. The axes chosen are

$$\begin{aligned}
&[11\bar{1}] \,||\, \mathbf{a}_1,\ a_1 = \tfrac{1}{2}\sqrt{3}A_1;\\
&[1\bar{1}0] \,||\, \mathbf{a}_2,\ a_2 = \sqrt{2}A_2;\ A_1 = A_2 = A_3 = A;\\
&[112] \,||\, \mathbf{a}_3,\ a_3 = \sqrt{6}A_3;
\end{aligned}$$

where a_1, A_1 etc. are written for the moduli of the vectors. Then

$$\begin{aligned}
\mathbf{a}_1 &= \tfrac{1}{2}\mathbf{A}_1+\tfrac{1}{2}\mathbf{A}_2-\tfrac{1}{2}\mathbf{A}_3\,,\\
\mathbf{a}_2 &= \mathbf{A}_1-\mathbf{A}_2+0\,,\\
\mathbf{a}_3 &= \mathbf{A}_1+\mathbf{A}_2+2\mathbf{A}_3\,,
\end{aligned}$$

and

$$\begin{aligned}
H &= \tfrac{1}{2}h+\tfrac{1}{2}k-\tfrac{1}{2}l\,,\\
K &= h-k\,,\\
L &= h+k+2l\,.
\end{aligned}$$

Table 1 gives the orthorhombic indices corresponding to the first six b.-c.c. powder pattern lines.

(2) *Calculation of X-ray intensities*

Consider a crystal consisting of M identical planes parallel to (112) planes stacked parallel to each other at a distance $\mathbf{a}_3/6$ and displaced parallel to each other as necessitated by the structure and by the distribution of faults present.

The Fourier transform T of the crystal is

$$T = \varphi\sum_n \exp\left[2\pi i\left(\delta_n a_1 s_1+(-1)^n(a_2/4)s_2+(na_3/6)s_3\right)\right], \quad (1)$$

where φ = transform of one layer,

s_1, s_2, s_3 are components of a reciprocal-lattice vector along a_1^*, a_2^*, a_3^* reciprocal-lattice axes, defined in the usual way,

δ_n = displacement of nth layer along $\mathbf{a}_1$.

The term $(-1)^n(a_2/4)s_2$ takes into account the displacement in the b.-c.c. structure of successive layers along $\mathbf{a}_2$.

If the diameter of the layers is large, φ has sharp maxima at $s_1 = Ha_1^*$, $s_2 = Ka_2^*$, where H, K are integers, and the transform consists of rods in reciprocal space along $\mathbf{a}_3$, passing through (H, K).

Writing $s_3 = \zeta a_3^*$,

$$T = \varphi\sum_n \exp\left[2\pi i\left(\delta_n H+(-1)^n K/4+n\zeta/6\right)\right]. \quad (2)$$

The intensity, therefore, is

$$\begin{aligned}
I(\zeta) = |\varphi|^2 \sum_n\sum_m \exp\big[2\pi i\big\{&(\delta_n-\delta_m)H\\
&+\left((-1)^n-(-1)^m\right)K/4+(n-m)\zeta/6\big\}\big]\,. \quad (3)
\end{aligned}$$

Putting $n' = n-m$, and summing over n for a given n',

$$\begin{aligned}
I(\zeta) = |\varphi|^2 \sum_{n'=-(M-1)}^{+(M-1)} &(-1)^{Kn'}(M-|n'|)\\
&\langle\exp\left[2\pi i\delta_{n'}H\right]\rangle \exp\left[2\pi i n'\zeta/6\right], \quad (4)
\end{aligned}$$

where $\delta_{n'} = \delta_n-\delta_m$ and $\langle\exp[2\pi i\delta_{n'}H]\rangle$ is the average value of $\exp[2\pi i\delta_{n'}H]$ over all n. Since the layers can take up three possible positions along $\mathbf{a}_1$, we write

$$\begin{aligned}
&\langle\exp\left[2\pi i\delta_{n'}H\right]\rangle\\
&\quad = A_{n'}+B_{n'}\exp\left[2\pi iH/3\right]+C_{n'}\exp\left[-2\pi iH/3\right], \quad (5)
\end{aligned}$$

where $A_{n'}, B_{n'}, C_{n'}$, are the probabilities of the n'th layers being at the A, B, C positions relative to the first layer. These probabilities are the same as for the f.-c.c. case, as calculated by Paterson (1952) and Wilson (1949) and others.

(3) *Deformation faults*

$$\left.\begin{aligned}
A_{n'} &= \tfrac{1}{3}+\tfrac{2}{3}(-1)^{n'}.[1-3\alpha(1-\alpha)]^{\frac{n'}{2}}.\cos n'\theta\,,\\
B_{n'} &= \tfrac{1}{3}-\tfrac{2}{3}(-1)^{n'}.[1-3\alpha(1-\alpha)]^{\frac{n'}{2}}.\cos\left(n'\theta+\tfrac{1}{3}\pi\right),\\
C_{n'} &= \tfrac{1}{3}-\tfrac{2}{3}(-1)^{n'}.[1-3\alpha(1-\alpha)]^{\frac{n'}{2}}.\cos\left(n'\theta-\tfrac{1}{3}\pi\right),
\end{aligned}\right\} \quad (6)$$

where α = stacking fault probability and $\tan\theta = \sqrt{3}(1-2\alpha)$. It follows from equations (4), (5) and (6) that for $H = 3N\pm1$, where N is an integer,

$$\begin{aligned}
I(\zeta) = |\varphi|^2\Big\{M+2\sum_1^{M-1}&(M-n')[1-3\alpha(1-\alpha)]^{\frac{n'}{2}}\\
&\times\cos 2\pi n'\left(\frac{\zeta}{6}+\frac{K+1}{2}\pm\frac{2\pi}{\theta}\right)\Big\}, \quad (7)
\end{aligned}$$

the positive and negative signs applying when $H = 3N+1$ and $3N-1$ respectively.

For $H = 3N$,

$$I(\zeta) = |\varphi|^2\left\{M+2\sum_1^{M-1}(M-n')\cos 2\pi n'\left(\frac{\zeta}{6}+\frac{K}{2}\right)\right\}. \quad (8)$$

Thus, reflexions with $H = 3N$ are unaffected by the faulting, and those with $H = 3N\pm1$ are broadened

into streaks along $\mathbf{a}_3^*$, exactly as in the f.-c.c. case. The peaks of these reflexions occur at $\zeta = 6N' \mp 3\theta/\pi - 3(K+1)$ and are therefore displaced from the corresponding positions in an unfaulted crystal by

$$d\zeta = \pm(1-3\theta/\pi) \simeq \pm\frac{3\sqrt{3}}{2\pi}\alpha \quad \text{(when } \alpha \text{ small)}$$

for $H = 3N \pm 1$. In principle, therefore, the probability of deformation faulting could be determined from the displacements of the lines, as in the f.-c.c. case†. The Fourier coefficients of the diffraction lines due to particle size and stacking faults are identical with those due to deformation faults in f.-c.c. structures, and methods similar to those used by Warren & Warekois (1955) could, at least in principle, be used to analyse the diffraction patterns in terms of strains, faults and particle size.

(4) *Line broadening*

The integral breadth is given by

$$\beta = \frac{\text{total intensity in line, } I_t}{\text{peak intensity, } I_p} .$$

On the ζ scale $I_t(\zeta) = 6MC$ and

$$I_p(\zeta) = M^2C \quad \text{for } h = 3N , \tag{9a}$$

$$I_p(\zeta) = \left[M + \frac{2r}{(1-r)^2}\{r^M - rM + M - 1\}\right]C$$
$$\text{for } h = 3N \pm 1, \text{ and } \alpha \neq 0 \text{ or } 1 \tag{9b}$$
$$\simeq M\frac{(1+r)}{(1-r)}C \quad \text{for large } M,$$

where

$$r = [1-3\alpha(1-\alpha)]^{\frac{1}{2}}, \text{ and } C = \int |\varphi|^2 ds_1 ds_2 .$$

If α is small,

$$I_p(\zeta) = \frac{4M}{3\alpha}C \text{ and } \beta_\zeta = \frac{9}{2}\alpha . \tag{10}$$

On the s scale ($s = 2\sin\theta/\lambda$, θ = Bragg angle, λ = wavelength),

$$I_t(s) = 6Ma_3^*C, \; I_p(s) = \frac{s}{\zeta a_3^*} I_p(\zeta)$$

and therefore

$$\beta_s = 6Ma_3^*C\Big/\frac{s}{\zeta a_3^*} I_p(\zeta) . \tag{11}$$

In powder photographs from randomly orientated crystals, several reflexions contribute to the same line; the resultant broadening is equal to the total intensity divided by the peak of the compound lines. In Table 1 the reflexions are arranged in 'broadened' and 'unbroadened' groups. It is clear that some of the reflexions, e.g. 200 and 310, should be exceptionally broad if stacking-fault broadening is important. In order to calculate the resultant broadening of each line we proceed as follows. For small α the breadths of the components are always greater than their displacements, for

$$\frac{\beta_\zeta}{d\zeta} = \frac{9\alpha/2}{3\sqrt{3}\alpha/2\pi} = \sqrt{3}\pi = 5{\cdot}44 . \tag{12}$$

It seems reasonable, therefore, to neglect the peak shifts to a first approximation. Then the broadening is given by

$$\beta_s = \Sigma 6MC\Big/sa_3^2 \Sigma \frac{I_p(\zeta)}{\zeta} ,$$

the sum being taken over all component lines. This expression is unsatisfactory for reflexions with $\zeta = 0$; for these the broadening due to the finite diameter of the layers, i.e. of the crystal, must be taken into account. These lateral dimensions of the crystals should also be considered for all the other reflexions which are not affected by the faulting. In order to arrive at a simple and consistent method of allowing for the finite size of the crystals for these reflexions, it will be assumed that the crystals are spherical, of radius R, and that the volume of the sphere is equal to the volume of the cylindrical crystal considered for the broadened reflexions. Further, it will be assumed that the latter cylindrical crystals have a diameter $Ma_3/6$

Table 1. *Corresponding b.-c.c. (hkl) and orthorhombic (HKL) indices*

hkl	*HKL*		*hkl*	*HKL*	
110	102		220	204	
$10\bar{1}$	$11\bar{1}$	B^*	202	$22\bar{2}$	B
$01\bar{1}$	$1\bar{1}\bar{1}$		022	$2\bar{2}\bar{2}$	
$1\bar{1}0$	020		$2\bar{2}0$	040	
101	013	S^*	202	026	S
011	$0\bar{1}3$		022	$0\bar{2}6$	
200	122		310	224	
020	$1\bar{2}2$	B	130	$2\bar{2}4$	
002	$\bar{1}04$		$3\bar{1}0$	142	
			$1\bar{3}0$	$\bar{1}4\bar{2}$	
$11\bar{2}$	$20\bar{2}$		103	$\bar{1}17$	
$21\bar{1}$	211		013	$1\bar{1}7$	
$12\bar{1}$	$2\bar{1}1$		$0\bar{1}3$	$\bar{2}15$	B
$2\bar{1}\bar{1}$	$13\bar{1}$		$10\bar{3}$	215	
$1\bar{2}1$	$\bar{1}31$	B	301	$13\bar{5}$	
211	115		031	$1\bar{3}5$	
121	$1\bar{1}5$		$30\bar{1}$	231	
$1\bar{1}2$	$\bar{1}24$		$03\bar{1}$	$2\bar{3}1$	
$1\bar{1}\bar{2}$	$12\bar{4}$				
112	006		222	108	
$2\bar{1}1$	$03\bar{3}$	S	$2\bar{2}2$	$\bar{1}44$	B
$12\bar{1}$	$03\bar{3}$		$\bar{2}22$	$1\bar{4}4$	
			$22\bar{2}$	300	S

* B: broad; S: sharp.

† However, as Prof. Warren pointed out (private communication), the average displacement of a line consisting of several different components, as calculated in a manner similar to that used for α-brass, turns out to be zero. This result is due to O. Guentert, whose work will be published shortly.

Table 2. *Average integral breadths of powder lines from crystals containing deformation faults*

		Numerical estimates of β_s for		
hkl	β_s	$\alpha M = 10$	$\alpha M = 100$	$\alpha M \gg 1$
110	$\left[\frac{5}{9}\sqrt{2}+\left(\frac{3}{2}\right)^{\frac{1}{3}}\frac{\sqrt{6}}{16}\alpha M\right]^{-1}\frac{\alpha}{A}$	$0{\cdot}394\frac{\alpha}{A}$	$0{\cdot}0546\frac{\alpha}{A}$	$\left(\frac{2}{3}\right)^{\frac{1}{3}}\frac{16}{\sqrt{6}}\frac{1}{MA}$
200	$0{\cdot}9\frac{\alpha}{A}$	$0{\cdot}9\frac{\alpha}{A}$	$0{\cdot}9\frac{\alpha}{A}$	$0{\cdot}9\frac{\alpha}{A}$
211	$\left[\frac{3}{5}\sqrt{6}+\left(\frac{3}{2}\right)^{\frac{1}{3}}\frac{\sqrt{6}}{32}\alpha M\right]^{-1}\frac{\alpha}{A}$	$0{\cdot}426\frac{\alpha}{A}$	$0{\cdot}0977\frac{\alpha}{A}$	$\left(\frac{2}{3}\right)^{\frac{1}{3}}\frac{32}{\sqrt{6}}\frac{1}{MA}$
220	$\left[\frac{5}{9}\sqrt{2}+\left(\frac{3}{2}\right)^{\frac{1}{3}}\frac{\sqrt{6}}{16}\alpha M\right]^{-1}\frac{\alpha}{A}$	$0{\cdot}394\frac{\alpha}{A}$	$0{\cdot}0546\frac{\alpha}{A}$	$\left(\frac{2}{3}\right)^{\frac{1}{3}}\frac{16}{\sqrt{6}}\frac{1}{MA}$
310	$0{\cdot}62\frac{\alpha}{A}$	$0{\cdot}62\frac{\alpha}{A}$	$0{\cdot}62\frac{\alpha}{A}$	$0{\cdot}62\frac{\alpha}{A}$
222	$\left[\frac{5}{12}\sqrt{3}+\left(\frac{3}{2}\right)^{\frac{1}{3}}\frac{\sqrt{6}}{32}\alpha M\right]^{-1}\frac{\alpha}{A}$	$0{\cdot}626\frac{\alpha}{A}$	$0{\cdot}105\frac{\alpha}{A}$	$\left(\frac{2}{3}\right)^{\frac{1}{3}}\frac{32}{\sqrt{6}}\frac{1}{MA}$

equal to their length. Equating the volumes of the two types of crystal assumed, gives

$$\frac{4}{3}\pi R^3 = \frac{\pi}{4}\left(\frac{Ma_3}{6}\right)^3,$$

and hence

$$R = \left(\frac{3}{2}\right)^{\frac{1}{3}}\cdot\frac{Ma_3}{12}.$$

As before, the total intensity on the s scale for a reflexion from the spherical crystal is $I_t(s) = 6Ma_3^{*}C$; whence, using the result derived by Wilson (1949) for the broadening due to small spherical crystals, we have

$$I_p(s) = \tfrac{3}{2}RI_t(s) = \tfrac{3}{4}\left(\tfrac{3}{2}\right)^{\frac{1}{3}}M^2C$$

and

$$\beta_s = \frac{\sum 6Ma_3^{*}}{sa_3\sum_b I_p(\zeta)/\zeta C+\sum_u \frac{3}{4}\left(\frac{3}{2}\right)^{\frac{1}{3}}M^2}, \qquad (13)$$

the two sums in the denominater being taken over the broadened ($\sum_b$) and unbroadened ($\sum_u$) reflexions respectively. Table 2 gives the calculated boradenings as a function of α, M and A. Numerical values for $\alpha M = 10$ and 100 are also given. It is clear from these results that the breadths of the 200 and 310 reflexions can be much greater than those of the other reflexions when stacking-fault broadening is important.

(5) *Growth faults*

For growth faults, if $0 < \alpha < (2\sqrt{3}-3)$,

$$A_{n'} = \frac{1}{3}-\frac{(-1)^{n'-1}(1-2\alpha)^{(n'-1)/2}}{3\sin\theta}\times[\sin n'\theta-2(1-2\alpha)^{\frac{1}{2}}\sin(n'-1)\theta],$$

$$B_{n'} = C_{n'} = \tfrac{1}{2}(1-A_{n'}), \qquad (14)$$

$$\tan\theta = -\frac{\sqrt{(3-6\alpha-\alpha^2)}}{(1-\alpha)}.$$

It follows that, for $H = 3N\pm1$,

$$I(\zeta) = |\varphi|^2\left\{M+\sum_1^{M-1}(M-n')(1-2\alpha)^{n'/2}\times\left[\cos 2\pi n'\left(\frac{\zeta}{6}+\frac{(K+1)}{2}+\frac{\theta}{2\pi}\right)-\frac{\alpha}{\sqrt{(3-6\alpha-\alpha^2)}}\sin 2\pi n'\left(\frac{\zeta}{6}+\frac{(K+1)}{2}+\frac{\theta}{2\pi}\right)+\cos 2\pi n'\left(\frac{\zeta}{6}+\left(\frac{K+1}{2}\right)-\frac{\theta}{2\pi}\right)+\frac{\alpha}{\sqrt{(3-6\alpha-\alpha^2)}}\sin 2\pi n'\left(\frac{\zeta}{6}+\frac{(K+1)}{2}-\frac{\theta}{2\pi}\right)\right]\right\}. \qquad (15)$$

For $(2\sqrt{3}-3) < \alpha < 1$ similar expressions can be obtained, using the methods developed by Paterson (1952) and in this paper. However, it is not clear whether a high density of faults is ever likely to occur in practice; when $\alpha = 1$ in the f.-c.c. structure the h.c.p. structure results; in the b.-c.c. case however, an orthorhombic structure would be produced, in which certain atoms are closer than in the original b.-c.c. structure. Such a structure seems improbable; further, since such short interatomic distances are produced at every fault (see Fig. 1), a high density of faults is unlikely. Similar considerations apply in the case of deformation faults.

For $H = 3N$,

$$I(\zeta) = |\varphi|^2\left\{M+\sum_1^{M-1}(M-n')\cos 2\pi n'\left(\zeta+\frac{K}{2}\right)\right\}, \qquad (16)$$

which is of course identical with the corresponding expression worked out for deformation faults.

Maxima of the broadened reflexions occur at

$$\zeta = 6N-3(K+1)\pm3\theta/\pi; \qquad (17)$$

the reflexions are displaced by

Table 3. *Average integral breadths of powder lines from crystals containing growth faults*

		Numerical estimates of β_s for		
hkl	β_s	$\alpha M = 10$	$\alpha M = 100$	$\alpha M \gg 1$
110	$\left[\frac{5}{12}\sqrt{2}+\left(\frac{3}{2}\right)^{\frac{1}{3}}\frac{\sqrt{6}}{16}\alpha M\right]^{-1}\frac{\alpha}{A}$	$0{\cdot}427\frac{\alpha}{A}$	$0{\cdot}0552\frac{\alpha}{A}$	$\left(\frac{2}{3}\right)^{\frac{1}{3}}\frac{16}{\sqrt{6}}\frac{1}{MA}$
200	$1{\cdot}2\frac{\alpha}{A}$	$1{\cdot}2\frac{\alpha}{A}$	$1{\cdot}2\frac{\alpha}{A}$	$1{\cdot}2\frac{\alpha}{A}$
211	$\left[\frac{9}{20}\sqrt{6}+\left(\frac{3}{2}\right)^{\frac{1}{3}}\frac{\sqrt{6}}{32}\alpha M\right]^{-1}\frac{\alpha}{A}$	$0{\cdot}505\frac{\alpha}{A}$	$0{\cdot}101\frac{\alpha}{A}$	$\left(\frac{2}{3}\right)^{\frac{1}{3}}\frac{32}{\sqrt{6}}\frac{1}{MA}$
220	$\left[\frac{5}{12}\sqrt{2}+\left(\frac{3}{2}\right)^{\frac{1}{3}}\frac{\sqrt{6}}{16}\alpha M\right]^{-1}\frac{\alpha}{A}$	$0{\cdot}427\frac{\alpha}{A}$	$0{\cdot}0552\frac{\alpha}{A}$	$\left(\frac{2}{3}\right)^{\frac{1}{3}}\frac{16}{\sqrt{6}}\frac{1}{MA}$
310	$0{\cdot}827\frac{\alpha}{A}$	$0{\cdot}827\frac{\alpha}{A}$	$0{\cdot}827\frac{\alpha}{A}$	$0{\cdot}827\frac{\alpha}{A}$
222	$\left[\frac{5}{16}\sqrt{3}+\left(\frac{3}{2}\right)^{\frac{1}{3}}\frac{\sqrt{6}}{32}\alpha M\right]^{-1}\frac{\alpha}{A}$	$0{\cdot}705\frac{\alpha}{A}$	$0{\cdot}108\frac{\alpha}{A}$	$\left(\frac{2}{3}\right)^{\frac{1}{3}}\frac{32}{\sqrt{6}}\frac{1}{MA}$

$$d\zeta = \pm\left(1+\frac{3\theta}{\pi}\right) \fallingdotseq \pm\frac{\sqrt{3}}{2\pi}\alpha^2 \quad \text{for small } \alpha.$$

For small α these displacements are negligible and cannot be observed; in this respect the effect of growth faults differs from that due to deformation faults. The total intensity on the ζ scale is again $6MC$. For $H = 3N \pm 1 (\alpha \neq 0)$,

$$I_p(\zeta) = \left[M+\frac{r}{(1-r)^2}\{r^M - rM + M - 1\}\right]C,$$

where $r = (1-2\alpha)^{\frac{1}{3}}$. For small α, $I_p(\zeta) = (M/\alpha)C$ and $\beta_\zeta = 6\alpha$. Also $\beta_\zeta/d\zeta = 4\sqrt{3}\pi/\alpha$, so that for small α, $d\zeta$ is always negligible compared with β_ζ. Therefore, making the same assumptions as in the case of deformation faults, the average broadening β_s on the s scale is obtained from expression (13), where $I_p(\zeta) = (M/\alpha)C$. Table 3 gives the results for growth faults. Again, the 200 and 310 reflexions should be exceptionally broad.

Discussion

The calculations show that the effect of stacking faults on the diffraction patterns from b.-c.c. crystals is similar to that in f.-c.c. crystals. In principle, oscillation techniques might be used to test for the presence of stacking faults, but the large multiplicity of 112 planes in the b.-c.c. case, i.e. 12, as compared with 4 in the f.-c.c. case might result in the masking of the effect on the X-ray photographs. It appears from the calculations that a study of the line broadening or of line shapes might be fruitful.

The diffraction lines from martensite are known to be very broad. Both Smith (1953), who examined low carbon (0·10–0·35%C) steels, and Wheeler & Jaswon (1947), who examined 1·35%C steels, noted that the 200 line is considerably broader than the neighbouring diffraction lines. In the former case, this exceptional broadening may be due to a slight tetragonality of the steels, which would lead to a relatively greater broadening of the 200 lines. A tetragonality corresponding to about 0·25%C has been measured by the use of special techniques (Roberts, Averbach & Cohen, 1953). This explanation cannot, however, account for a similar anomaly in the Wheeler & Jaswon experiments, in which the 200+020 line could be separated from the 002 line. Since a considerable part of the broadening is due to strains (Smith, 1953), it was suggested that the anomaly might be due to the relatively small value of Young's modulus in the [100] direction compared to that in the [110] or [211] directions. Both Wheeler & Jaswon and Smith noted, however, that the ratios of the Young's moduli were rather greater than necessary to explain the anomaly, if it is assumed that the stresses rather than the strains are independent of crystallographic direction. It is possible, however, that the anomaly may be due to stacking faults, and it is interesting to re-interpret the results on this basis. Fig. 2 shows Smith's values of $\beta\cos\theta$ plotted as a function of $\sin\theta$. The points for the 110, 211 and 220 reflexions lie close to a straight line through the origin, from the slope of which the average root-mean-square strain ($\frac{1}{4}\beta\cot\theta$) is found to be 0·0058; the height of the point from the 200 reflexion above the line corresponds to a deformation stacking fault probability $\alpha = 0{\cdot}009$, i.e. one fault every 130 Å ($\sim$ 110 (211) planes). This estimate is based on the assumption that faults occur only on one set of (112) planes in the crystal; it is possible that faults occur simultaneously on several sets of planes. Supposing that faults occur on three sets of planes the average distance between faults is 390 Å; this may be taken as the average distance ($2R$) between partial dislocations. Assuming that the root-mean-square strain of this set of dislocations is $\sim\langle b\rangle/R$, where $\langle b\rangle$ is the average Burgers vector of the partial dislocations at the ends of the stacking faults and equal to $\frac{3}{2}.A/2\sqrt{3}$,

its value is found to be about 0·0069, which is of the same order as the root-mean-square strain determined from the slope of the straight line. Similar agreement was obtained by Warren & Warekois (1955) in their analysis of cold-worked α-brass.

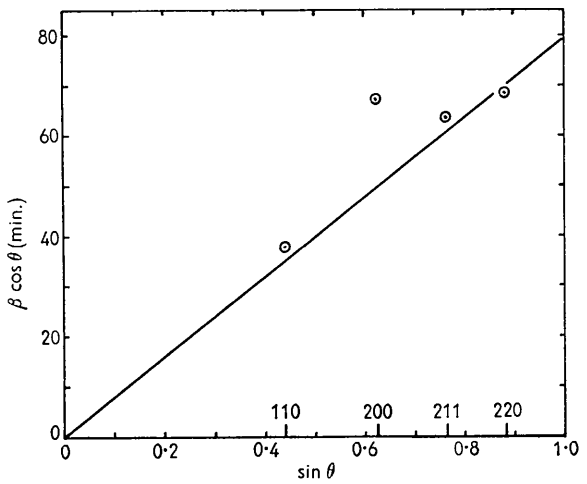

Fig. 2. Variation of $\beta \cos \theta$ with $\sin \theta$ for a low-carbon martensite (Smith, 1953).

With regard to the possibility of the production of faults by deformation, the results of Smallman (1953) on the line broadening from iron filings are of interest. Once again, the 200 reflexion is exceptionally broad, and, if this discrepancy is explained in terms of stacking faults as above, α is found to be 0·002, i.e. one fault every 585 Å. The root-mean-square strain would be $\sim 0{\cdot}0015$ compared to the values 0·0032 and 0·0041 determined experimentally by Smallman for two types of iron filed at room temperature. Using Mo $K\alpha$ radiation, several high-order lines could be studied, and the results show that the 200, 310 and 400 lines are exceptionally broad. These observations could be explained on the assumption of stacking faults (see Table 2), but also in terms of the anisotropy of the elastic constants.

This discussion should be regarded as purely speculative in view of the lack of more precise experimental data, and in view of the fact that the anomalies can be explained in other ways. The results obtained, however, suggest that evidence for stacking faulting might be obtained from more extensive measurements of line shapes.

Part of this work was carried out during the summer of 1955 at the University of Illinois, and the authors wish to thank Prof. T. A. Read for his interest in this work and for providing the necessary facilities. P. B. H. wishes to thank Prof. N. F. Mott and Dr W. H. Taylor (Cavendish Laboratory, Cambridge) for their interest and encouragement, and the University of Illinois for the award of the George Miller Visiting Professorship. H. M. O. wishes to thank Prof. G. V. Raynor for facilities, and the Managers of the I. C. I. Fellowship Fund for the award of a Fellowship. The authors would like to acknowledge a useful discussion with Prof. B. E. Warren while this work was being completed.

References

Barrett, C. S. (1949). *The Cold Working of Metals*, p. 65. Cleveland: American Society of Metals.

Barrett, C. S. (1950). *Phase Transformations in Solids*. New York: Wiley.

Barrett, C. S. (1952). *Imperfections in Nearly Perfect Crystals*. New York: Wiley.

Barrett, C. S. (1956). *Acta Cryst.* **9**, 671.

Cahn, R. W. (1954). *Advances in Phys.* **3**, 363.

Cottrell, A. H. (1953). *Dislocations and Plastic Flow*, pp. 76 and 86 ff. Oxford: Clarendon Press.

Cottrell, A. H. & Bilby, B. A. (1951). *Phil. Mag.* (7), **42**, 573.

Edwards, O. S. & Lipson, H. (1942). *Proc. Roy. Soc.* A, **180**, 268.

Frank, F. C. & Nicholas, J. F. (1953). *Phil. Mag.* (7), **44**, 1213.

Hirsch, P. B., Kelly, A. & Menter, J. W. (1955). *Proc. Phys. Soc.* B, **68**, 1132.

Kelly, A. (1953). *Proc. Phys. Soc.* A, **66**, 403.

Paterson, M. S. (1952). *J. Appl. Phys.* **23**, 805.

Paxton, H. W. (1953). *Acta Metallurg.* **1**, 141.

Roberts, C. S., Averbach, B. L. & Cohen, M. (1953). *Trans. Amer. Soc. Met.* **45**, 576.

Smallman, R. E. (1953). Ph.D. Dissertation, University of Birmingham, England.

Smith, R. A. (1953). *J. Iron Steel Inst.* **173**, 147.

Suzuki, H. (1954). *Sci. Rep. Res. Insts. Tohoku Univ.* A, **6**, 30.

Warren, B. E. & Warekois, E. P. (1955). *Acta Metallurg.* **3**, 473.

Wechsler, M. S., Lieberman, D. S. & Read, T. A. (1953). *Trans. Amer. Inst. Min. (Metall.) Engrs.* **197**, 1503.

Wheeler, J. A. & Jaswon, M. A. (1947). *J. Iron Steel Inst.* **157**, 161.

Wilson, A. J. C. (1949). *X-ray Optics*. London: Methuen.