based on any other fault-structure for the crystal would agree as well with the observations.

Finally we wish to record our appreciation of the help and advice we have had from Prof. Bragg and Dr Perutz.

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A Note on Deformation Stacking Faults in Hexagonal Close-Packed Lattices

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Formulae for the intensity distribution in reciprocal space, and for the integrated intensity and integral breadth of a diffraction maximum, are given for a h.c.-p. structure containing a random distribution of deformation faults.

1. Introduction

The effect of faults in the stacking of the close-packed layers of the f.-c.c and h.c.-p. lattices has been discussed by several authors, especially Wilson (1942, 1949) and Paterson (1952). The diffraction effects depend on the origin of the faults; in particular a distinction has been drawn between 'growth' and 'deformation' faulting (Barrett, 1952). More complex stacking sequences ('extrinsic faults') are also possible (Frank & Nicholas, 1953), but probably have higher energy.

The faulting parameter, α, is defined as the fractional area of all atomic close-packed planes which are faulted. The dissociation of lattice dislocations in close-packed planes gives some faults even in well annealed crystals, but these are insufficient to produce observable diffraction effects. Extensive faulting may be produced by mechanical deformation, martensitic transformation and (possibly) atomic growth. Consideration of the first two of these processes suggests that only deformation faults in both lattices, and h.c.-p. growth faults are likely to be important in practice. Formulae have previously been given for growth faulting in h.c.-p. lattices and for both types of faulting in f.-c.c. lattices. In this note, we give the corresponding formulae for h.c.-p. deformation faulting.

2. Intensity distribution in reciprocal space

We use the same notation as Paterson (1952), except that α is the h.c.-p. faulting parameter, and our vector $\mathbf{a}_3$ is equal to the interplanar translation, so that the factor $\frac{1}{3}h_3$ in his expressions is replaced by h_3. The intensity distribution for $H-K = 3N\pm1$ may then be written

$$I(HKh_3) = C[J_0+\sum_1^\infty \{J_m \exp 2\pi i m h_3+(J_m \exp 2\pi i m h_3)^*\}]$$

and

$$J_m = f^2[P^0_m-\tfrac{1}{2}(P^+_m+P^-_m)\pm i\sqrt{3}\,.\tfrac{1}{2}.(P^+_m-P^-_m)]\,.$$

A difference equation for the probabilities P_m may be obtained by considering possible sequences of planes in a manner similar to that used by Paterson. This equation is

$$P^0_m-P^0_{m-2}(1-3\alpha+3\alpha^2) = \alpha-\alpha^2$$

and has solution

$$P^0_m = \tfrac{1}{3}+\frac{2\varrho-1}{6\varrho}\varrho^m+\frac{2\varrho+1}{6\varrho}(-\varrho)^m,$$

where $\varrho = +(1-3\alpha+3\alpha^2)^{\frac{1}{2}}$ and is always real.

Similarly

$$P^+_m = P^-_m = \tfrac{1}{3}+\frac{1-2\varrho}{12\varrho}\varrho^m-\frac{1+2\varrho}{12\varrho}(-\varrho)^m.$$

From this we find

$$J_m = f^2\varrho^m\left[\frac{2\varrho-1}{4\varrho}+(-1)^m\frac{2\varrho+1}{4\varrho}\right],$$

and the intensity distribution in reciprocal space is represented by

$$I(HKh_3) = f^2C\left[1+\sum_1^\infty \varrho^m\left\{\frac{2\varrho-1}{2\varrho}\cos 2\pi m h_3 + \frac{2\varrho+1}{2\varrho}\cos 2\pi m(h_3+\tfrac{1}{2})\right\}\right]$$

$$= f^2C\left[\frac{(2\varrho-1)(1-\varrho^2)}{4\varrho(1-2\varrho\cos 2\pi h_3+\varrho^2)} + \frac{(2\varrho+1)(1-\varrho^2)}{4\varrho(1-2\varrho\cos 2\pi(h_3+\frac{1}{2})+\varrho^2)}\right]. \quad (1)$$

The first part of this expression has a peak value of $(2\varrho-1)(1+\varrho)/4\varrho(1-\varrho)$ when $h_3 = L$ (an integer), and the second part a peak value of $(2\varrho+1)(1+\varrho)/4\varrho(1-\varrho)$ when $h_3 = L+\frac{1}{2}$. These maxima are in the positions of the maxima from a perfect h.c.-p. lattice, so there is no shift of peak position whatever the value of α.

If we suppose the crystal to be a small parallelepiped having M_1, M_2, M_3 unit cells in the directions of $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$, the total number of atoms is $M = M_1M_2M_3$, and $C = M^2/M_3$. The integrated intensity obtained from any region of reciprocal space round a maximum is

$$T = \int_{h_1}\int_{h_2}\int_{h_3} I(h_1h_2h_3)dh_1dh_2dh_3 = \frac{1}{M_1M_2}\int_{h_3} I(HKh_3)dh_3 .$$

The integrated intensities of the two parts of equation (1) may thus be written

$$T_e = Mf^2\int_{L-\frac{1}{2}}^{L+\frac{1}{2}} \frac{(2\varrho-1)(1-\varrho^2)}{4\varrho(1-2\varrho\cos 2\pi h_3+\varrho^2)}dh_3 = Mf^2\frac{2\varrho-1}{4\varrho} ,$$

$$T_0 = Mf^2\frac{2\varrho+1}{4\varrho} .$$

For $\alpha = 0$ or $\alpha = 1$, these have the values $Mf^2/4$, $3Mf^2/4$ characteristic of the perfect h.c.-p. lattice. As α increases intensity is transferred from the lines with maxima at $h_3 = L$ to the others, until at $\alpha = \frac{1}{2}$ the first part of the intensity expression becomes zero, and there is only one set of maxima.

The integral breadth of a line is defined by

$$B = \frac{\int I(HKh_3)\,dh_3}{I(HKh_3)_{\mathrm{Max.}}}$$

and we find for both sets of lines that

$$B = \frac{1-\varrho}{1+\varrho} = \frac{2-3\alpha(1-\alpha)-2(1-3\alpha+3\alpha^2)^{\frac{1}{2}}}{3\alpha(1-\alpha)} .$$

It is noteworthy that the integral breadths of the lines in a deformation-faulted h.c.-p. crystal are identical with those in a similarly faulted f.-c.c. crystal (Paterson, 1952). The maximum breadth ($B = \frac{1}{3}$) is obtained at $\alpha = \frac{1}{2}$, when only the $h_3 = L+\frac{1}{2}$ components remain.

3. Measurement of α

F.-c.c. crystals containing either deformation or growth stacking faults give X-ray diffraction photographs which show a shift in the position of the maxima when compared with the unfaulted crystal. This method provides the most convenient way of detecting the presence of such faults, but is not available for h.c.-p. materials, where J_m is always real, and the peak positions are unaffected. The value of α may then be determined by measurement of integrated intensities, integral breadths or line shapes. The latter method, developed by Warren & Averbach (1952), is probably the best way of obtaining the maximum information from any one line. Its use becomes very tedious, however, when a large number of specimens have to be examined, and for ordinary work the measurement of line breadths seems to be almost as accurate.

Comparison of the above results with those previously obtained for growth faulting shows that while the effects are similar, the type of faulting can readily be determined. In both cases intensity is transferred from the even lines to the odd lines, until at $\alpha = \frac{1}{2}$ only the odd lines remain and have integral breadth $\frac{1}{3}$. In growth faulting, however, the ratio $B_0/B_e = \frac{1}{3}$ exactly, whereas in deformation faulting $B_0 = B_e$. A further difference lies in the rate at which the intensity is transferred. For growth faulting, $T_0/T_e = 3{\cdot}35$ for $\alpha = 0{\cdot}3$, whereas for deformation faulting $T_0/T_e = 3{\cdot}82$ for $\alpha = 0{\cdot}1$ and $10{\cdot}23$ for $\alpha = 0{\cdot}3$. Providing the diffraction broadening due to faulting can be satisfactorily separated from that due to other causes, it is therefore possible to determine the predominant type of faulting and measure its frequency quite accurately.

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