SHORT COMMUNICATIONS

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Acta Cryst. (1979). A**35**, 337–338

The diffraction of X-rays by face-centred cubic crystals containing extrinsic stacking faults – a derivation from the general theory.

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(*Received* 7 *August* 1978; *accepted* 6 *September* 1978)

Abstract

A solution is given to that problem of extrinsic faulting in face-centred cubic crystals in which additional layers may be inserted after layers of the original crystal or, generally with a different probability, after previously inserted layers. Two previous results are deduced as special cases.

In a previous paper (Howard, 1977) the following model for a face-centred cubic crystal containing extrinsic faults was considered. Given first the original crystal with original layers in the usual stacking sequence for a face-centred cubic crystal, we allow the consecutive addition of any number of inserted layers after any original layer. We suppose that an original layer is followed by an inserted layer with probability p while an inserted layer is followed by another inserted layer with probability q. With $q = 0$ this model leads to the diffraction problem solved by Johnson (1963), while with $q = p$ the model gives the problem attempted by Sabine (1966) and solved by Howard (1977) [hereafter referred to as (I)]. The present model was introduced in (I) in the discussion where it was concluded that a solution *via* a difference equation was clearly possible but the difference equation might have an order as high as eight. Furthermore, it seemed that the more general theories of diffraction by faulted crystals might not be applicable to a problem of this kind. Under these circumstances, in (I), no solution for the present model was attempted.

It was recognized by one of us (NK) that the above problem was not beyond the scope of general theory, and indeed we demonstrate in this note how the theory of Kakinoki & Komura (1965) is applied in this case. The intensity distribution derived here reduces, as required, to the results given previously by Johnson (1963) and in (I) for the cases $q = 0$ and $q = p$ respectively.

We suppose, as usual, that the stacking sequence in the original face-centred-cubic crystal is $ABCABC\cdots$, but we shall identify these original layers as A_0, B_0, C_0. We have to distinguish two types of inserted layer: A_1 denotes an inserted layer which, if the original sequence is resumed, is followed by C_0, while A_2 denotes an inserted layer which would be followed on resumption of the original sequence by B_0. We use B_1, B_2, C_1, C_2, in an analogous manner. With this notation, some examples of possible sequences are:

$A_0B_0C_0A_0\cdots$	(the original crystal),
$A_0B_0A_1C_0A_0\cdots$	(a single inserted layer),
$A_0B_0A_1B_2C_0A_0\cdots$	(two successive inserted layers),
$A_0B_0A_1B_2A_1C_0A_0\cdots$	(three successive inserted layers).

The model under consideration may be described by listing the probabilities in a **P** table of the type given by Kakinoki (1967). In Table 1 we list the distinct followed layers down the side, and the distinct following layers across the top. In the body of the table we enter the relevant probabilities. The **P** table has the same dimensions as Table 14 of Kakinoki (1967).

Table 1. *The complete* **P** *table*

	A_0	A_1	A_2	B_0	B_1	B_2	C_0	C_1	C_2
A_0				$1-p$				p	
A_1						q	$1-q$		
A_2				$1-q$				q	
B_0		p					$1-p$		
B_1	$1-q$								q
B_2		q					$1-q$		
C_0	$1-p$				p				
C_1			q	$1-q$					
C_2	$1-q$				q				

The diffraction may now be calculated with the methods given by Kakinoki (1967). We give a brief outline, following precisely the notation, the steps and the formulae of that paper.

Step 1:

$$\mathbf{P}_1 = \begin{pmatrix} 1-p & 0 & 0 \\ 0 & 0 & q \\ 1-q & 0 & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{P}_2 = \begin{pmatrix} 0 & p & 0 \\ 1-q & 0 & 0 \\ 0 & q & 0 \end{pmatrix}$$

Step 2:

$$w_0 = \frac{1-q^2}{1-q^2+p+pq}; \; f_{A_0} = f_{B_0} = f_{C_0} = w_0/3,$$

$$w_1 = \frac{p}{1-q^2+p+pq}; \; f_{A_1} = f_{B_1} = f_{C_1} = w_1/3,$$

$$w_2 = \frac{pq}{1-q^2+p+pq}; \; f_{A_2} = f_{B_2} = f_{C_2} = w_2/3.$$

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Step 3:

$$T_m = \frac{1}{1-q^2+p+pq} \times \text{spur}\begin{pmatrix} 1-q^2 & p & pq \\ 1-q^2 & p & pq \\ 1-q^2 & p & pq \end{pmatrix}\begin{pmatrix} (1-p)\varepsilon & p\varepsilon^* & 0 \\ (1-q)\varepsilon^* & 0 & q\varepsilon \\ (1-q)\varepsilon & q\varepsilon^* & 0 \end{pmatrix}^m;$$

therefore

$$T_1 = [(pq-2p) + (1-3p-q^2+3pq)\varepsilon]/(1-q^2 + p + pq),$$

$$T_2 = [(-1+4p-3p^2-2pq+q^2+3p^2q) - (1-3p - q^2+3pq)\varepsilon]/(1-q^2+p+pq).$$

Step 4:

$$F(x) = \begin{vmatrix} x-(1-p)\varepsilon & -p\varepsilon^* & 0 \\ -(1-q)\varepsilon^* & x & -q\varepsilon \\ -(1-q)\varepsilon & -q\varepsilon^* & x \end{vmatrix} = 0,$$

$$a_1 = -(1-p)\varepsilon,$$
$$a_2 = -q^2 - p(1-q)\varepsilon,$$
$$a_3 = -q(p-q)\varepsilon.$$

Step 5 with formula (3):

$$C_0 = 2 - 2p + 2p^2 - 2p^2q - pq^2 + q^4 + pq^3 + p^2q^2 + q^2(p-q)^2,$$

$$C_1 = 1 - pq - p^2 + 2p^2q - pq^2 + q^4 - p^2q^2 + (1-p+q^2-q^2p-q^3p+q^4)\varepsilon,$$

$$C_2 = p - 2q^2 - qp^2 + q^2p + (p-pq)\varepsilon,$$

$$C_3 = q(p-q)(1+\varepsilon),$$

$$E_0 = 3p[1-p^2-pq+5p^2q-2pq^2 - p^3q - 3p^2q^2 + 3pq^3 - q^4 + p^3q^2 - p^2q^3 + (-1+2p+q-p^2+q^2 - 4pq + 4p^2q - q^3 + 3pq^3 - 4p^2q^2 + p^2q^3 - pq^4)\varepsilon]/(1-q^2+p+pq),$$

$$E_1 = 3p[q(p-q)(-1-p+q+pq) + (1-p-q+2pq - p^2q + p^2q^2 - pq^3)\varepsilon]/(1-q^2+p+pq),$$

$$E_2 = 3pq(1-q)(p-q)/(1-q^2+p+pq),$$

$$D_0 = 3p(2-2p-q+2pq+2p^2q - 2pq^2 - 2p^2q^2 + pq^3 + pq^4 - q^5)/(1-q^2 + p + pq),$$

$$D_1 = 3p[q(p-q)(-1-p+q+pq) + (1-p-q + pq + q^2 - q^3)\varepsilon]/(1-q^2+p+pq),$$

$$D_2 = E_2,$$

and the intensity is given by

$$D(\varphi) = \{D_0 + [D_1\exp(i\varphi) + D_2\exp(2i\varphi) + \text{complex conjugate}]\} \times \{C_0 + [C_1\exp(i\varphi) + C_2\exp(2i\varphi) + C_3\exp(3i\varphi) + \text{complex conjugate}]\}^{-1}$$

Rather than give a detailed discussion of the form of the above distribution, we verify that it reduces to known solutions in special cases. For $q=0$ we obtain

$$C_0 = 2(1-p+p^2),$$
$$C_1 = (1-p)(1+p+\varepsilon) = (1-p)(p-\varepsilon^*),$$
$$C_2 = p(1+\varepsilon) = -p\varepsilon^*, \quad C_3 = 0,$$
$$D_0 = 6p(1-p)/(1+p),$$
$$D_1 = 3p(1-p)\varepsilon/(1+p), \quad D_2 = 0,$$

and it can be seen by comparison with equation (50) of Kakinoki (1967) that we have obtained the Johnson (1963) result. For $q=p$ we obtain

$$C_0 = 2-2p+2p^2-3p^3+3p^4,$$
$$C_1 = (1-p)[1+p-p^2+(1+p^2)\varepsilon],$$
$$C_2 = p-2p^2+(p-p^2)\varepsilon, \quad C_3 = 0,$$
$$D_0 = 3p(1-p)(2-p+p^2+p^3)/(1+p),$$
$$D_1 = 3p(1-p)(1-p+p^2)\varepsilon/(1+p), \quad D_2 = 0.$$

So for $q=p$:

$$D_\pm(\varphi) = \frac{3p(1-p)}{1+p} \times [2-p+p^2+p^3+2(1-p+p^2)\cos(\varphi \pm 2\pi/3)] \times [2-2p+2p^2-3p^3+3p^4+2(1-p)(1+p-p^2)\cos\varphi + 2p(1-2p)\cos 2\varphi + 2(1-p)(1+p^2)\cos(\varphi \pm 2\pi/3) + 2p(1-p)\cos(2\varphi \pm 2\pi/3)]^{-1}$$

where (Kakinoki, 1967) the upper and lower signs correspond to the cases $h-k=3n+1$ and $h-k=3n-1$ respectively. With $\varphi = \pi l$, it can be shown that this expression is identical to expression (14) for intensity appearing in (I).

In an independent study Takahashi (1978) has also recognized that the results in (I) could be derived from the general theory. His results are evidently equivalent to ours, and he shows graphically examples of intensity profiles for $q=0$, for $q=p$, and for $q=(1+p)/2$.

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