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A note on *On the diffraction of X-rays by face-centred cubic crystals containing extrinsic stacking faults* by C. J. Howard.

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The intensity of X-ray scattering from f.c.c. crystals containing extrinsic stacking faults with two fault parameters [see Howard (1977). *Acta Cryst.* A**33**, 29–32] has been calculated.

Howard (1977) has recently calculated the intensity of X-rays diffracted from an f.c.c. crystal containing extrinsic stacking faults by a method using difference equations (Holloway & Klamkin, 1969). He has also given a more general model for faulting with two fault parameters, p and q, but no solution has been given. In this note, the intensity formula for the above two-parameter model is derived by using the matrix method given by Kakinoki (1967).

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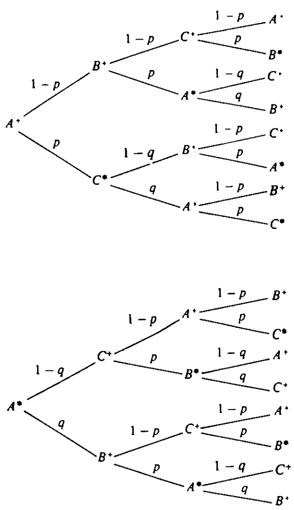

Fig. 1. The stacking sequence of layers for the two-parameter model given by Howard (1977). Analogous probability trees can be drawn from B^+, B^*, C^+ and C^*.

Table 1. *The* '**P**-*table*' *representing the same stacking sequence as that shown in Fig.* 1

		A^+	A^*	B^+	B^*	C^+	C^*
$w/3$	A^+			$1-p$			p
$w'/3$	A^*			q		$1-q$	
$w/3$	$B+$		p			$1-p$	
$w'/3$	B^*	$1-q$				q	
$w/3$	C^+	$1-p$			p		
$w'/3$	C^*	q		$1-q$			

Fig. 1 shows the probability trees obtained on the basis of Howard's two-parameter model. According to Kakinoki (1967), the stacking sequence of layers shown in Fig. 1 can be represented by the '**P**-table' as shown in Table 1, where $w = 1/(1+p)$ and $w' = p/(1+p)$, $w/3$ and $w'/3$ being probabilities of occurrence of layers in a crystal of types A^+ (B^+ or C^+) and A^* (B^* or C^*) respectively. The intensity formula for the diffuse scattering can then easily be derived as follows:

$$I = \frac{P_0[P_1 - 2P_2\cos\pi(l \mp \frac{1}{3})]}{Q_0 + Q_1\cos\pi l \pm Q_2\sin\pi l + Q_3\cos 2\pi l \pm Q_4\sin 2\pi l} \quad (1)$$

where the hexagonal coordinates $[hk.l]$ are the same as those of Howard; the upper and lower signs correspond to the cases $(h-k)\equiv 1 (\mathrm{mod}\ 3)$ and $(h-k)\equiv 2 (\mathrm{mod}\ 3)$ respectively; $P_0 = 3p(1-p+pq)/(1+p)$, $P_1 = 2-q-pq$, $P_2 = 1-q$, $Q_0 = 2(1-p+p^2) - 3p^2q(1-q)$, $Q_1 = (1-p)(1+2p-3pq)$, $Q_2 = -\sqrt{3}(1-p)(1+pq)$, $Q_3 = p(1-3q)$ and $Q_4 = -\sqrt{3}p(1-q)$.

For $q = p$, equation (1) reduces to

$$I = \frac{3p(1-p)(1-p+p^2)[2+p-2\cos\pi(l \mp \frac{1}{3})]/(1+p)}{A} \quad (2)$$

with

$$\begin{aligned} A = {} & 2(1-p+p^2) - 3p^3(1-p) + (1-p)^2(1+3p) \\ & \times \cos\pi l \mp \sqrt{3}(1-p)(1+p^2)\sin\pi l \\ & + p(1-3p)\cos 2\pi l \mp \sqrt{3}p(1-p)\sin 2\pi l \end{aligned}$$

which is identical with equation (14) of Howard, though these two equations have apparently quite different forms. For $q = 0$, an equation the same as that given by Johnson [1963; see equation (15) of Howard] can be obtained.

References

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