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X-RAY DIFFRACTION FROM THE 8H(44) STRUCTURE CONTAINING STACKING FAULTS

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The influence of all possible 23-types of faults in the 8H(44) structure on peak broadening $\Delta w\{h_3\}$, peak shifts $\Delta h_3\{h_3\}$, and changes in the intensity of the peak maxima was estimated for single crystal reflexions with h_3 == 8M, 8M±1, ±2, ±3, ±4. The values of $\Delta h_3\{h_3\}$,, $\Delta w\{h_3\}$ and $I_{max}(h_3)$ were calculated using the same expressions as in the previous paper. The coefficients a_i *of* the characteristic equation and the boundary conditions, *J(m),* were calculated by the Prasad and Leie method, which was adopted in this paper to the 8H(44) structure and other long periodic nH(n/2 n/2)-type structures. On the basis of the results obtained, the new method of stacking faults analysis in the above structures was presented. The results for 8H(44) structure was compared with the theoretical intensity distributions, $I_{10.l}$ which we obtained by the model analysis method. Moreover, some examples of the stacking faults analysis in the ZnSe doping Mn crystals with 8H(44) structure were presented.

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/. *Introduction*

The theory presented by Michalski et al. (1980), in the previous paper, is illustrated here by some examples of calculations for the 8H(44) structure. The usefulness of the expressions for $\Delta h_3(h_3)$, $\Delta w(h_3)$ and $I_{max}(h_3)$ obtained in the previous paper is shown. On the basis of these results the corollaries which were possible to involve are presented in terms of the new method of the stacking faults analysis. In the calculations some simplifications and generalizations for nH(n/2 n/2) structures are introduced.

The characteristic symmetry in D_m and N_m (used in the previous paper) and its connection with the method of the characteristic equation coefficients calculation and boundary conditions are illustrated.

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2. *Stacking faults in 8H(44) structure*

Let the succeeding layers in each of three sequences (starting with A_O, B_O or C_o) of a perfect 8H(44) structure be denoted by subscripts j (j = 0. 1. .... 7). Thus this crystal can be represented by the following layers;

$$A_0 \quad B_1 \quad C_2 \quad A_3 \quad B_4 \quad A_5 \quad C_6 \quad B_7$$

$$B_0 \quad C_1 \quad A_2 \quad B_3 \quad C_4 \quad B_5 \quad A_6 \quad C_7$$

$$C_0 \quad A_1 \quad B_2 \quad C_3 \quad A_4 \quad C_5 \quad B_6 \quad A_7 \qquad (1)$$

Thus the 24-types of layers (8-types of A_j, B_j and C_j) could be distinguished by different sequences of the next layers. In the perfect 8H(44) structure starting with A_o only the following layers A_o, B_1, C_2, A_3, B_4, A_5, C_6 and B_7 with succession shown by subscripts j can occur. Other types of layers or another succession of layers can occur only by the formation of stacking faults. To describe all possible types of faults it is necessary and sufficient to take into consideration after each layer, one perfect layer or 8 faulted layers. For example, after the B_1 - layer the C_2 -layer can occur followed by no fault and $A_o, \ldots, A_7$ - layers followed by different types of faults.

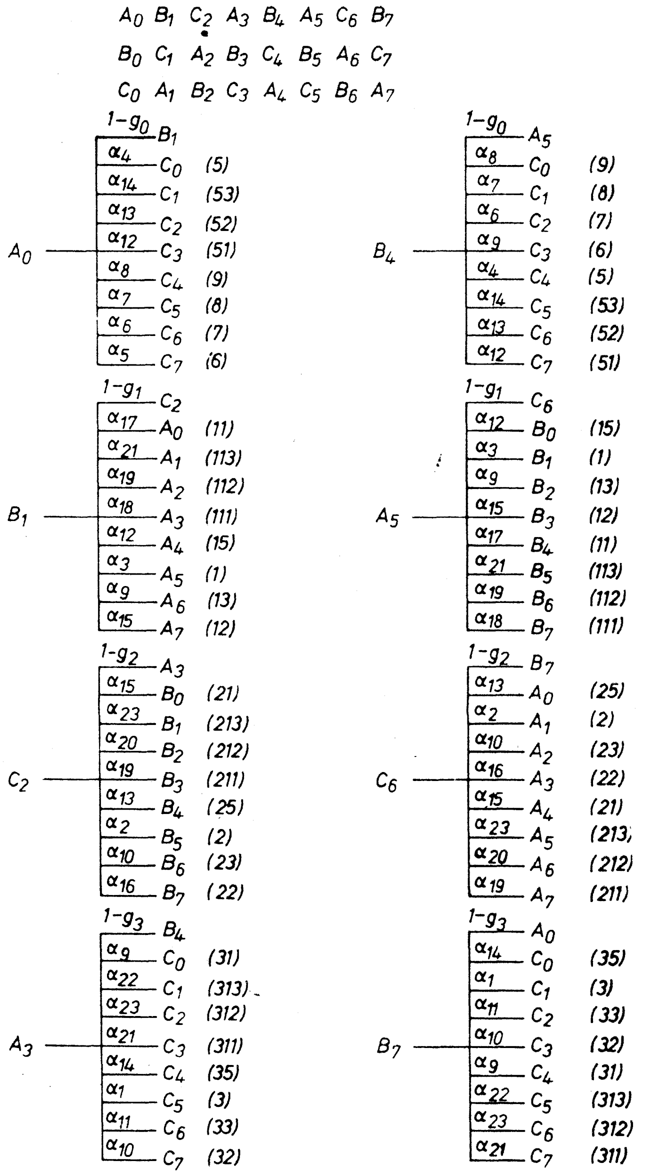
The probability trees for successive layers of the sequence starting with A_o are presented in Fig. 1. Symbols $(1 - g_j)$ mark probabilities of the occurrence of layers followed by no faults. Symbols α_i, denote probabilities of the occurrence of *i*-types of faults. In the brackets Zhdanov's symbols for the corresponding faults are given. Zhdanov's symbols, used for describing the faults, are more useful for interpretation and generalization of obtained results than Jagodzinski's *hk* symbols used by Prasad and Leie (1970).

3. *Recurrence relation for P(m,j)*

Following Prasad and Leie (1970) let $P(m,j)$ be the probability of finding of an m-th layer with a particular value of j in the sequence having ${}^1k$ faults of type 1, ${}^2k$ faults of type 2, ..., ${}^{23}k$ faults of type 23. Let the $P(m,j,{}^ik-1)$ be a probability of that occurrence in the sequence having the number of faults type "*i*" less by the one than in the previous sequence. From Fig. 1 it is seen that the *m*-layer with subscript $j = 0$ can be formed in the following nine ways:

— from the $(m-1)$ -layer with $j = 7$ occurring with probability $P(m-1, 7)$ followed by no fault with probability $(1-g_3)$,

— from the $(m-1)$-layers with j = 7, 6, 5, 4, 3, 2, 1 and 0 occurring with probabilities $P(m-1, 7, {}^{14}k-1)$, $P(m-1, 6, {}^{13}k-1)$, $P(m-1, 5, {}^{12}k-1)$, $P(m-1, 4, {}^{8}k-1)$, $P(m-1, 3, {}^{9}k-1)$, $P(m-1, 2, {}^{15}k-1)$, $P(m-1, 1, {}^{17}k-1)$ and $P(m-1, 0, {}^{4}k-1)$ respectively, followed by fault type 14, 13, 12, 8, 9, 15, 17 and 4 occurring with probabilities α_{14}, α_{13}, α_{12}, α_8, α_9, α_{15}, α_{17} and α_4.



$$g_0 = \alpha_4 + \alpha_{14} + \alpha_{13} + \alpha_{12} + \alpha_8 + \alpha_7 + \alpha_6 + \alpha_5 \quad g_0' = \alpha_4 + \alpha_{14} + \alpha_{13} + \alpha_{12}, \quad g_0'' = \alpha_8 + \alpha_7 + \alpha_6 + \alpha_5$$

$$g_1 = \alpha_{17} + \alpha_{22} + \alpha_{19} + \alpha_{18} + \alpha_{12} + \alpha_3 + \alpha_9 + \alpha_{15}, \quad g_1' = \alpha_{17} + \alpha_{22} + \alpha_{19}, \quad g_1'' = \alpha_{12} + \alpha_3 + \alpha_9 + \alpha_{15}, \quad g_1''' = \alpha_{18}$$

$$g_2 = \alpha_{15} + \alpha_{23} + \alpha_{20} + \alpha_{19} + \alpha_{13} + \alpha_2 + \alpha_{10} + \alpha_{16}, \quad g_2' = \alpha_{15} + \alpha_{23} + \alpha_{20} + \alpha_{19}, \quad g_2'' = \alpha_{13} + \alpha_2 + \alpha_{10}; \quad g_2''' = \alpha_{16}$$

$$g_3 = \alpha_9 \cdot \alpha_{22} + \alpha_{23} + \alpha_{21} + \alpha_{14} + \alpha_1 + \alpha_{11} + \alpha_{10}, \quad g_3' = \alpha_9 + \alpha_{22} + \alpha_{23} + \alpha_{21}, \quad g_3'' = \alpha_{14} + \alpha_1 + \alpha_{11} + \alpha_{10}$$

Fig. l. Probability trees for successive layers of 8H(44) structure starting with A_o

The probability $P(m, 0)$ of obtaining the m-th layer with $j = 0$ is a sum of the nine above events probabilities and so we have

$$P(m, 0) = (1-g_3)P(m-1, 7)+\alpha_{14}P(m-1, 7, {}^{14}k-1)+\alpha_{13}P(m-1, 6, {}^{13}k-1)$$
$$+\alpha_{12}P(m-1, 5, {}^{12}k-1)+\alpha_8 P(m-1, 4, {}^{8}k-1)+\alpha_9 P(m-1, 3, {}^{9}k-1)$$
$$+\alpha_{15}P(m-1, 2, {}^{15}k-1)+\alpha_{17}P(m-1, 1, {}^{17}k-1)+\alpha_4 P(m-1, 0, {}^{4}k-1). \quad (2)$$

Similarly we can express the remaining $P(m,j)$.

4. Discussion of a phase

Stacking faults can (as it is seen in Fig. 1) produce changes of layer subscripts j and changes of their symbols A, B or C in relation to those occurring in the sequences followed by no fault. The phase change of a wave diffracted by an m-layer can be studied in two steps, fn the first step we only consider the effect of a change of layer subscript j while preserving its belonging to the sequence starting at A_O. The change of subscript j with layer phase (the place of a layer A, B or C) in sequence starting with A_O, can be expressed as follows:

j	0	1	2	3	4	5	6	7	8
$F(j)$	0	f_o	$-f_o$	0	f_o	0	$-f_o$	f	0

(3)

In the second step we consider the displacements of layers in the plane parallel to the layers of about $\pm s$ ($s = 1/6$ [1010]) with respect to the layers having the same j in the sequence followed by no fault and starting with A_O. The effect of the value j for layers obtained by fault on the layer displacement (0, $+s$, $-s$) is presented in Table I.

Let the K_p denote the sum of ${}^{i}k_j$ numbers of i-type faults producing layer displacements with subscript j by $+s$ and K_n producing $-s$ displacement. Then, on the basis of Table I, we have

$$K_p = {}^{1}k_1+{}^{2}k_5+{}^{4}k_4+{}^{5}k_7+{}^{7}k_1+{}^{8}k_4+{}^{9}k_4+{}^{9}k_6+{}^{10}k_2+{}^{10}k_7+{}^{12}k_7+{}^{12}k_0$$
$$+{}^{14}k_1+{}^{14}k_4+{}^{15}k_0+{}^{15}k_3+{}^{19}k_3+{}^{19}k_2+{}^{20}k_6+{}^{21}k_7+{}^{21}k_5+{}^{22}k_1, \quad (4)$$
$$K_n = {}^{1}k_5+{}^{2}k_1+{}^{4}k_0+{}^{5}k_3+{}^{7}k_5+{}^{8}k_0+{}^{9}k_0+{}^{9}k_2+{}^{10}k_6+{}^{10}k_3+{}^{12}k_3+{}^{12}k_4+{}^{14}k_5$$
$$+{}^{14}k_0+{}^{15}k_4+{}^{15}k_7+{}^{19}k_7+{}^{19}k_6+{}^{20}k_2+{}^{21}k_3+{}^{21}k_1+{}^{22}k_5. \quad (5)$$

The general expression for the m-th layer phase with a given value *of* j can be expressed as

$$\Phi(m, j) = \Phi(j)+(K_p-K_n)\varphi_0. \quad (6)$$

To find a recurrence relation for $J(m,j)$, defined by

$$J(m, j) = \sum_k P(m, j)\exp[i\Phi(m, j)], \quad (7)$$

we have used the following relationships for phase difference. If a phase difference between waves diffracted by the *m'th* and origin layers in a sequence containing less by one number

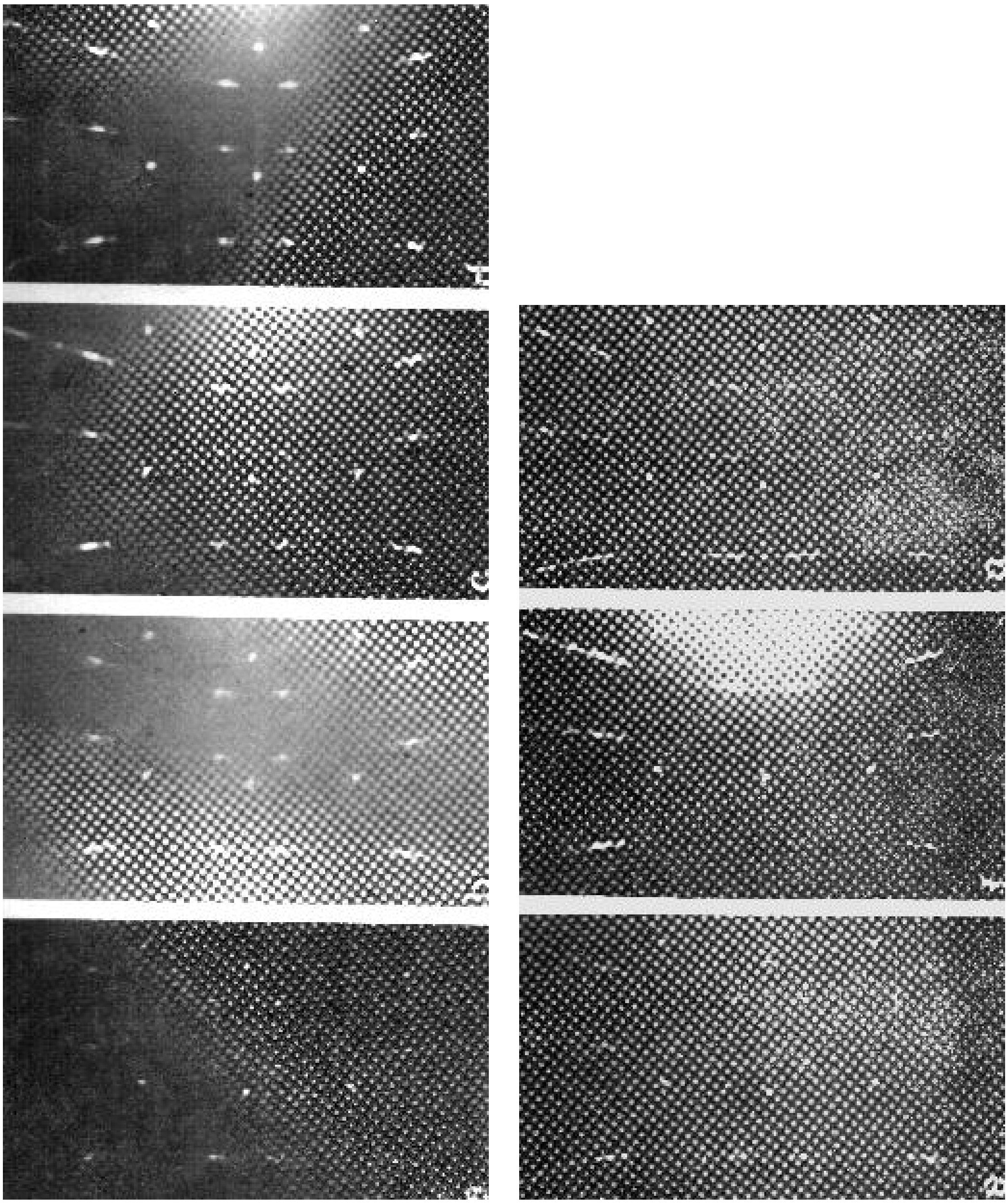


Fig. 2. The 10.l, 11.l and 20.l rows of X-ray diffraction photographs (a rotation of a crystal about the c-axis) of Mn-doping ZnSe (a, b, c, d, e and f) and In-doping ZnS (g) crystals

TABLE I

The dependence of shift (0, $+s$, $-s$) on the value of the subscript j for layers formed as a result of particular faults

Fault			Value of j for displacement through		
			$+S$	$-S$	0
1	(3)	A_3C_5 B_7C_1	1	5	
2	(2)	C_2 B_5, C_6 A_1	5	1	
3	(1)	B_1 A_5, A_5 B_1			1,5
4	(5)	A_0 C_0, B_4 C_4	4	0	
5	(6)	A_0 C_7 B_4 C_3	7	3	
6	(7)	A_0 C_6 B_4 C_2			6,2
7	(8)	A_0C_5 B_4 C_1	1	5	
8	(9)	A_0 C_4, B_4 C_0	4	0	
9	(31) (13)	A_3 C_0, B_7 C_4 B_1 A_6 A_5 B_2	4,6	0,2	
10	(23) (32)	C_2 B_6, C_6 A_2 A_3 C_7, B_7 C_3	2,7	6,3	
11	(33)	A_3 C_6, B_7 C_2			6,2
12	(51) (15)	A_0 C_3, B_4 C_7 B_1 A_4, A_5 B_0	7,0	3,4	
13	(52) (25)	A_0 C_2, B_4 C_6 C_2 B_4, C_6 A_0			6,2,4,0
14	(53) (35)	A_0 C_1, B_4 C_5 A_3 C_4, B_7 C_0	1,4	5,0	
15	(21) (12)	C_2 B_0, C_6 A_4 B_1 A_7, A_5 B_3	0,3	4,7	
16	(22)	C_2 B_7, C_6 A_3			7,3
17	(11)	B_1 A_0, A_5 B_4			0,4
18	(111)	A_1 B_3 A_5 B_7			7,3
19	(211) (112)	C_2 B_3, C_6 A_7 B_1 A_2, A_5 B_6	3,2	7,6	
20	(212)	C_2 B_2 C_6 A_6	6	2	
21	(311) (113)	A_3 C_3, B_7 C_7 B_1 A_1 A_5 B_5	7,5	3,1	
22	(313)	A_3 C_1 B_7 C_5	1	5	
23	(312) (213)	A_3C_2 B_7 C_6 C_2 B_1, C_6 A_5			2,6,1,5

of some fault which involve $+s$ displacement, the phase difference will be equal to $(K_p-1-K_n)\phi_o$. However, for less by one number of some fault, which involve $-s$ displacement, the phase difference will be equal to $(K_p-K_n+1)\phi_o$.

5. *Recurrence relation for J(m,j)*

Let us first consider $J(m, 0)$. According to Prasad and Leie (1970) it can be expressed in the following manner:

$$J(m,0) = \sum_k P(m,0)\exp[i\Phi(m,0)] = \sum_k [(1-g_3)P(m-1,7)+\alpha_{14}P(m-1,7,{}^{14}k-1)$$
$$+\alpha_{13}P(m-1,6,{}^{13}k-1)+\alpha_{12}P(m-1,5,{}^{12}k-1)+\alpha_8 P(m-1,4,{}^{8}k-1)$$
$$+\alpha_9 P(m-1,3,{}^{9}k-1)+\alpha_{15}P(m-1,2,{}^{15}k-1)+\alpha_{17}P(m-1,1,{}^{17}k-1)$$
$$+\alpha_4 P(m-1,0,{}^{4}k-1)]\exp[i\varphi_0(K_p-K_n)].$$

Let us rearrange the terms in the above equation to obtain after each of $P(m-l,j)$ on the right side of this equation of adequate $\exp[i\Phi(m-1,j)]$ multiplied by $\exp(i\phi_o) = \exp(2/3\pi i)$ or $\exp(-i\phi_o) = \exp(-2/3\pi i)$. Here we have used equation (6), in which the first term of $\Phi(j)$ is determined by (3) while the second by Table I.

$$J(m,0) = (1-g_3)\sum P(m-1,7)\exp[i\varphi_0\{1+(K_p-K_n)\}]\exp(-i\varphi_0)$$
$$+\alpha_{14}\sum P(m-1,7,{}^{14}k-1)\exp[i\varphi_0\{1+(K_p-K_n+1)\}]\exp(i\varphi_0)$$
$$+\alpha_{13}\sum P(m-1,6,{}^{13}k-1)\exp[i\varphi_0\{-1+(K_p-K_n)\}]\exp(i\varphi_0)$$
$$+\alpha_{12}\sum P(m-1,5,{}^{12}k-1)\exp[i\varphi_0(K_p-K_n+1)]\exp(i\varphi_0)$$
$$+\alpha_8\sum P(m-1,4,{}^{8}k-1)\exp[i\varphi_0\{1+(K_p-K_n+1)\}]\exp(i\varphi_0)$$
$$+\alpha_9\sum P(m-1,3,{}^{9}k-1)\exp[i\varphi_0(K_p-K_n+1)]\exp(-i\varphi_0)$$
$$+\alpha_{15}\sum P(m-1,2,{}^{15}k-1)\exp[i\varphi_0\{-1+(K_p-K_n-1)\}]\exp(-i\varphi_0)$$
$$+\alpha_{17}\sum P(m-1,1,{}^{17}k-1)\exp[i\varphi_0\{1+(K_p-K_n)\}]\exp(-i\varphi_0)$$
$$+\alpha_4\sum P(m-1,0,{}^{4}k-1)\exp[i\varphi_0\{(K_p-K_n+1)\}]\exp(-i\varphi_0).$$

Substituting the adequate $J(m-1,j)$ and $\omega = \exp(i\varphi_0) = \exp\left(\frac{2\pi}{3}i\right)$ or $\omega^2 = \exp(-i\varphi_0) = \exp\left(-\frac{2\pi}{3}i\right)$ on the right side of the above equation, we have

$$J(m,0) = (1-g_3)\omega^2 J(m-1,7)+\alpha_{14}\omega J(m-1,7)+\alpha_{13}\omega J(m-1,6)$$
$$+\alpha_{12}\omega J(m-1,5)+\alpha_8\omega J(m-1,4)+\alpha_9\omega^2 J(m-1,3)$$
$$+\alpha_{15}\omega^2 J(m-1,2)+\alpha_{17}\omega^2 J(m-1,1)+\alpha_4\omega^2 J(m-1,0)\,. \tag{8}$$

Similarly one can express the remaining $J(m,j)$ in terms of the following system of equations

$$J(m,j) = f_j[J(m-1,0),\ldots,J(m-1,n-1)]. \tag{9}$$

6. Characteristic equation

Let the solution of (9) have the form

$$J(m, j) = C_j \varrho^m, \tag{10}$$

where Cj and ρ are functions of α's.

Substituting this solution into (9), we obtain after some rearrangement

$$\begin{bmatrix}
\alpha_4\omega^2-\varrho & \alpha_{17}\omega^2 & \alpha_{15}\omega^2 & \alpha_9\omega^2 & \alpha_8\omega & \alpha_{12}\omega & \alpha_{13}\omega & (1-g_3)\omega^2+\alpha_{14}\omega \\
(1-g_0)\omega+\alpha_{14}\omega^2 & \alpha_{21}\omega^2-\varrho & \alpha_{23}\omega^2 & \alpha_{22}\omega^2 & \alpha_7\omega & \alpha_3\omega & \alpha_2\omega & \alpha_1\omega \\
\alpha_{13}\omega^2 & (1-g_1)\omega+\alpha_{19}\omega^2 & \alpha_{20}\omega^2-\varrho & \alpha_{23}\omega^2 & \alpha_6\omega & \alpha_9\omega & \alpha_{10}\omega & \alpha_{11}\omega \\
\alpha_{12}\omega^2 & \alpha_{18}\omega^2 & (1-g_2)\omega+\alpha_{19}\omega^2 & \alpha_{21}\omega^2-\varrho & \alpha_5\omega & \alpha_{15}\omega & \alpha_{16}\omega & \alpha_{10}\omega \\
\alpha_8\omega^2 & \alpha_{12}\omega^2 & \alpha_{13}\omega^2 & (1-g_3)\omega+\alpha_{14}\omega^2 & \alpha_4\omega-\varrho & \alpha_{17}\omega & \alpha_{15}\omega & \alpha_9\omega \\
\alpha_7\omega^2 & \alpha_3\omega^2 & \alpha_2\omega^2 & \alpha_1\omega^2 & (1-g_1)\omega^2+\alpha_{14}\omega & \alpha_{21}\omega-\varrho & \alpha_{23}\omega & \alpha_{22}\omega \\
\alpha_6\omega^2 & \alpha_9\omega^2 & \alpha_{10}\omega^2 & \alpha_{11}\omega^2 & \alpha_{13}\omega & (1-g_1)\omega^2+\alpha_{19}\omega & \alpha_{20}\omega-\varrho & \alpha_{23}\omega \\
\alpha_5\omega^2 & \alpha_{15}\omega^2 & \alpha_{16}\omega^2 & \alpha_{10}\omega^2 & \alpha_{12}\omega & \alpha_{18}\omega & (1-g_2)\omega^2+\alpha_{19}\omega & \alpha_{21}\omega-\varrho
\end{bmatrix}
\begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \\ C_7 \end{bmatrix} = 0 \tag{11}$$

For non-trivial values of the solutions, C_j, the determinant of the first matrix must vanish. Following the preliminary assumptions of this theory (small α's) we neglect all the terms which contain products of different α_i. Thus, the determinant of the above eight rows of the matrix can be substituted by the sum of 23 determinants calculated simply for particular $\alpha_i \neq 0$. In this manner, the condition of a non-trivial solution C_j can be expressed in terms of the following characteristic equation

$$a_8\varrho^8+a_7\varrho^7+a_6\varrho^6+a_5\varrho^5+a_4\varrho^4+a_3\varrho^3+a_2\varrho^2+a_1\varrho+a_0 = 0, \tag{12}$$

where the coefficients of α_j (after neglecting the terms having powers of a, greater than one) one can write

$$a_8 = 1, \quad a_7 = \alpha_4+\alpha_{20}+2\alpha_{21}, \quad a_6 = \alpha_5-2\alpha_{17}-4\alpha_{23}, \quad a_5 = -2\alpha_6+2\alpha_{15}+\alpha_{22},$$

$$a_4 = \alpha_7-2\alpha_9-2\alpha_{16}, \quad a_3 = -2\alpha_3+\alpha_8+2\alpha_{10}, \quad a_2 = \alpha_2-2\alpha_{11}+2\alpha_{12},$$

$$a_1 = \alpha_1-4\alpha_{13}-2\alpha_{18}, \quad a_0 = -1+2(\alpha_1+\alpha_2+\alpha_3+\alpha_4+\alpha_5+\alpha_6+\alpha_7+\alpha_8+2\alpha_9$$

$$+2\alpha_{10}+\alpha_{11}+2\alpha_{12}+2\alpha_{13}+3\alpha_{14}+2\alpha_{15}+\alpha_{16}+\alpha_{17}+\alpha_{18}+3\alpha_{19}+\alpha_{20}+2\alpha_{21}+\alpha_{22}+2\alpha_{23}).$$

7. *Boundary conditions*

Boundary conditions will be evaluated in two steps, using the method of Prasad and Leie (1970). First we obtain the probability w_j of finding a layer with a particular value of j, which passes through an arbitrary region of a crystal (arbitrary m). From Fig. 1 result the following relationships among particular w_j's

$$
\begin{aligned}
w_0 &= \alpha_4 w_0+\alpha_{17}w_1+\alpha_{15}w_2+\alpha_9 w_3+\alpha_8 w_4+\alpha_{12}w_5+\alpha_{13}w_6+(1-g_3+\alpha_{14})w_7,\\
w_1 &= (1-g_0+\alpha_{14})w_0+\alpha_{21}w_1+\alpha_{23}w_2+\alpha_{22}w_3+\alpha_7 w_4+\alpha_3 w_5+\alpha_2 w_6+\alpha_1 w_7,\\
w_2 &= \alpha_{13}w_0+(1-g_1+\alpha_{19})w_1+\alpha_{20}w_2+\alpha_{23}w_3+\alpha_6 w_4+\alpha_8 w_5+\alpha_{10}w_6+\alpha_{11}w_7,\\
w_3 &= \alpha_{12}w_0+\alpha_{18}w_1+(1-g_2+\alpha_{14})w_2+\alpha_{21}w_3+\alpha_5 w_4+\alpha_{15}w_5+\alpha_{16}w_6+\alpha_{10}w_7,\\
w_4 &= \alpha_8 w_0+\alpha_{12}w_1+\alpha_{13}w_2+(1-g_3+\alpha_{14})w_3+\alpha_4 w_4+\alpha_{17}w_5+\alpha_{15}w_6+\alpha_9 w_7,\\
w_5 &= \alpha_7 w_0+\alpha_3 w_1+\alpha_2 w_2+\alpha_1 w_3+(1-g_0+\alpha_{14})w_4+\alpha_{21}w_5+\alpha_{23}w_6+\alpha_{22}w_7,\\
w_6 &= \alpha_6 w_0+\alpha_9 w_1+\alpha_{10}w_2+\alpha_{11}w_3+\alpha_{13}w_4+(1-g_1+\alpha_{19})w_5+\alpha_{10}w_6+\alpha_{23}w_7,\\
w_7 &= \alpha_5 w_0+\alpha_{15}w_1+\alpha_{16}w_2+\alpha_{10}w_3+\alpha_{12}w_4+\alpha_{18}w_5+(1-g_2+\alpha_{19})w_6+\alpha_{21}w_7, \qquad (13)
\end{aligned}
$$

moreover the normalizing condition is

$$\sum_{j=0}^{7} w_i = 1. \qquad (14)$$

On the basis of the symmetry of (13) it can be found that: $w_o = w_4$, $w_1 = w_5$, $w_2 = w_6$ *and* $w_3 = w_7$. Thus, taking equations (13) and (14) the problem simplifies to solving 3 linear, nonhomogeneous equations

$$w_j a_{kj} = b_k, \qquad (15)$$

where k, j = 1, 2, 3 and the coefficients a_{kj} and b_k are linear functions of α_i probabilities. Using assumptions about α_i, (α_i are small ones) the solution of (15) can be written as

$$w_j = C_{0j}+\sum_i C_{ij}\alpha_i, \qquad (16)$$

where i = 1, 2, ..., 23 and j = 1, 2, 3.

The terms of C_{oj} (free of α_i) and coefficients C_{ij} were found by solving 24 very simple systems of 3 equations with 3 unknowns. For w_j we have obtained the following values:

$$
\begin{aligned}
w_1 = w_5 &= \tfrac{1}{8}[1+\tfrac{1}{4}(\alpha_1+2\alpha_2+3\alpha_3-\alpha_4-2\alpha_5-3\alpha_6-\alpha_8-8\alpha_{10}-2\alpha_{11}-2\alpha_{13}\\
&\quad +2\alpha_{15}+2\alpha_{17}+\alpha_{16}-\alpha_{20}+\alpha_{21}+\alpha_{22})],\\
w_2 = w_6 &= \tfrac{1}{8}[1+\tfrac{1}{4}(\alpha_1+2\alpha_2-\alpha_3-\alpha_4-2\alpha_5+\alpha_6-\alpha_8+4\alpha_{10}+2\alpha_{11}-4\alpha_{12}+2\alpha_{13}\\
&\quad -2\alpha_{15}-2\alpha_{17}-3\alpha_{18}+3\alpha_{20}-3\alpha_{21}+\alpha_{22}+4\alpha_{23})],\\
w_3 = w_7 &= \tfrac{1}{8}[1+\tfrac{1}{4}(\alpha_1-2\alpha_2-\alpha_3-\alpha_4+2\alpha_5+\alpha_6-\alpha_8+4\alpha_{10}+2\alpha_{11}-2\alpha_{13}+2\alpha_{15}\\
&\quad -2\alpha_{17}+\alpha_{18}-\alpha_{20}+\alpha_{21}+\alpha_{22})], \qquad (17)
\end{aligned}
$$

and using the condition (14)

$$w_0 = w_4 = \tfrac{1}{8}[1-\tfrac{1}{4}(3\alpha_1+2\alpha_2+\alpha_3-3\alpha_4-2\alpha_5-\alpha_6-3\alpha_8+2\alpha_{11}-4\alpha_{12}-2\alpha_{13}+2\alpha_{15}-2\alpha_{17}-\alpha_{18}+\alpha_{20}-\alpha_{21}+3\alpha_{22}+4\alpha_{23})].$$

Then, considering all the possible sequences starting with A_o, B_1, C_2, A_3, B_4, A_5, C_6 and B_7 one can directly calculate the values of $J(m) = \sum w_j$ <exp $[i\Phi(m,j)]$> for $m = 0, 1, ..., 7$. From Fig. 1 it can be seen, that

$$J(0) = \sum_{j=0}^{7} w_j \exp(0) = 1 \tag{18}$$

and

$$J(1) = \sum_{j=0}^{7} \tfrac{1}{8} w_j[\exp(+i\varphi_0)+\exp(-i\varphi_0)] = -\tfrac{1}{2}. \tag{19}$$

Further m calculations of $J(m)$ are more complicated because of the increasing number of terms which are terms of a geometric series. However, it can be seen that in each of the sequences after the $(m$~- 1)-layer two layers can occur, whose phases are both displaced with respect to origin layer by $\pm\ \phi_o$ (in opposite directions), or two m-layers of which the first layer will be identical to that of the origin one and the phase of the second layer displaced by $\pm\ \phi_o$. Probabilities of the occurrence of these layers are expressed by (1 —gj) or g_j, Moreover, the phase of the m-layer of the sequence starting with X_j (for which the probability of occurrence is determined by w_j) will be contrary to that of the sequence starting with $X_{j\pm4}$ (its probability of occurrence is determined by $w_{j\pm4} = w_j$). The probabilities of the occurrence of the (m-l)-layer are in these sequences equal. From this results the possibility of adding in <exp [$i\Phi(m,j)$]> the terms describing sequences starting with X_j and $X_{j\pm4}$. Therefore for each of sequences the last factor in <exp [$i\Phi(m,j)$]> will be expressed by one of the following terms

$$(1-g_j)[\exp(\pm i\varphi_0)+\exp(\mp i\varphi_0)]+g_j[\exp(\pm i\varphi_0)+\exp(\mp i\phi_0)] = -1,$$
$$(1-g_j)[\exp(\pm i\phi_0)+\exp(\mp i\varphi_0)]+g_j[\exp(0)+\exp(0)] = 3g_j-1,$$
$$(1-g_j)[\exp(0)+\exp(0)]+g_j[\exp(\pm i\varphi_0)+\exp(\mp i\varphi_0)] = 2-3g_j. \tag{20}$$

Using the above one can give the method of expressing the $J(m)$ by α_i which considerably simplifies the calculations, especially for large m. Let us write $J(m)$ as follows

$$J(m) = \sum_{j=0}^{3} w_j T_j, \tag{21}$$

where T_j are α_i functions determined as

$$T_j = (1-g_j)S_{j+1}+g_j^{\wedge}S_{j+2}+g_j^{\wedge\wedge}S_{j+2}^{-}, \quad \text{for} \quad j = 0, 3,$$
$$T_j = (1-g_j)S_{j+1}+g_j^{\wedge}S_{j-1}+g_j^{\wedge\wedge}S_{j+2}+g_j^{\wedge\wedge}S_j^{-}, \quad \text{for} \quad j = 1,$$
$$T_j = (1-g_j)S_{j+1}+g_j^{\wedge}S_{j-1}+g_j^{\wedge\wedge}S_{j-2}^{-}+g_j^{\wedge\wedge}S_{j+1}^{-}, \quad \text{for} \quad j = 2. \tag{22}$$

Denotations of $g_j^{\wedge}$ $g_j^{\wedge\wedge}$, $g_j^{\wedge\wedge\wedge}$ are in agreement with Fig. 1. The sign "-" upwards denotes the transition to second row in probability trees in Fig. 1. Because we want to take into consideration in *J(m)* terms with first power of a_i only, it is sufficient to determine free terms (without of a_i). According to (20) they can take values -1 or 2 depending on the last factor in <exp *iF(m,j)*]> for the considered sequence. However, the terms standing at the (1 —g_j) must be determined with an accuracy to the first power of a_i. We proceed by analogy to T_j. For example

$$S_{j+1} = 1-g_{j+1}R_{j+2}+g_{j+1}^{\wedge}R_{j+3}+g_{j+1}^{\wedge\wedge}R_{j+3}^{-}, \tag{23}$$

for $j+1 = 0, 3$.

Here it is necessary to determine R_{j+2} exactly, and free terms in R_{j+3} and R^{-}_{j+3}. After finding the exact value to the last factor (1—g_{j+m-2}), we successively substitute terms calculated to the corresponding (1 —*g*) up to T_j. In this way we express the remaining *J(m)* by a_i

$$J(2) = \tfrac{1}{32}[-4+3(\alpha_1+2\alpha_2+3\alpha_3-\alpha_4-2\alpha_5-3\alpha_6-4\alpha_7-5\alpha_8+8\alpha_{10}+2\alpha_{11}+4\alpha_{12} +2\alpha_{13}+14\alpha_{15}+4\alpha_{16}+6\alpha_{17}+9\alpha_{18}+16\alpha_{19}+13\alpha_{21}+5\alpha_{22}+12\alpha_{23})], \tag{24}$$

$$J(3) = \tfrac{1}{32}[8+6(-\alpha_1-2\alpha_2-\alpha_3+\alpha_4+4\alpha_5+3\alpha_6+4\alpha_7+5\alpha_8-4\alpha_9-6\alpha_{10}-4\alpha_{11} -2\alpha_{13}-6\alpha_{15}-4\alpha_{16}-2\alpha_{17}-3\alpha_{18}-8\alpha_{19}-5\alpha_{20}-3\alpha_{21}-3\alpha_{22}-8\alpha_{23})], \tag{25}$$

$$J(4) = \tfrac{1}{32}[-4+3(\alpha_1+6\alpha_2-5\alpha_3+3\alpha_4-6\alpha_5-3\alpha_6-4\alpha_7-5\alpha_8-4\alpha_9+8\alpha_{10}+2\alpha_{11} -4\alpha_{12}+10\alpha_{13}+4\alpha_{14}-6\alpha_{15}+12\alpha_{16}-2\alpha_{17}+\alpha_{18}+3\alpha_{20}-3\alpha_{21}+\alpha_{22}+4\alpha_{23})], \tag{26}$$

$$J(5) = \tfrac{1}{32}[8+6(-7\alpha_1-4\alpha_2+5\alpha_3+5\alpha_4+6\alpha_5+5\alpha_6+5\alpha_7+5\alpha_8+4\alpha_9-6\alpha_{10}-6\alpha_{11} +12\alpha_{12}+2\alpha_{13}-2\alpha_{14}-5\alpha_{15}-4\alpha_{16}+2\alpha_{17}+2\alpha_{19}-\alpha_{20}+\alpha_{21}-3\alpha_{22}-4\alpha_{23})], \tag{27}$$

$$J(6) = \tfrac{1}{32}[-4+3(21\alpha_1-6\alpha_2-9\alpha_3-5\alpha_4+6\alpha_5+9\alpha_6+8\alpha_7+7\alpha_8-4\alpha_9+16\alpha_{10} +22\alpha_{11}-16\alpha_{12}-10\alpha_{13}+16\alpha_{14}-10\alpha_{15}-4\alpha_{16}-2\alpha_{17}-11\alpha_{18}-4\alpha_{19}+3\alpha_{20}-3\alpha_{21} +5\alpha_{22}+8\alpha_{23})], \tag{28}$$

$$J(7) = \tfrac{1}{8}[-4+3(7\alpha_2+2\alpha_3+7\alpha_4+2\alpha_5+2\alpha_6+2\alpha_7+2\alpha_8+5\alpha_9+7\alpha_{10}+9\alpha_{12}+14\alpha_{13} +7\alpha_{14}+5\alpha_{15}+4\alpha_{16}+4\alpha_{17}+8\alpha_{18}+7\alpha_{19}+3\alpha_{20}+7\alpha_{21}+3\alpha_{22}+6\alpha_{23})]. \tag{29}$$

8. Estimation of the influence of stacking faults on the peak shifts, peak broadening and change of the peak maxima intensity

Following expression (2) of the previous paper the diffracted intensity from a faulted 8H(44) structure can be written as

$$I(h_3) = \psi^2 \left[1 + \frac{2\sum_{m=0}^{8} N_m \cos\frac{m\pi}{4} h_3}{\sum_{m=0}^{8} D_m \cos\frac{m\pi}{4} h_3} \right], \tag{30}$$

TABLE II

The effect of stacking faults on the shifts $\Delta h_3(h_3)$, broadenings $\Delta w(h_3)$ and changes in peak maxima intensity $I_{max}(h_3)$ for different single crystal reflexions

Zhdanov's symbols	h_3 \ a_i	$\Delta h_3[a_i]$					$\Delta w[a_i]$					$\frac{1}{\psi}2I_{max}\left[\frac{1}{a_i}\right]$				
		8M	8M±1	8M±2	8M±3	8M±4	8M	8M±1	8M±2	8M±3	8M±4	8M	8M±1	8M±2	8M±3	8M±4
3	a_1	0	$\mp\frac{\sqrt{2}}{4\pi}$	$\mp\frac{1}{2\pi}$	$\mp\frac{\sqrt{2}}{4\pi}$	0	$\frac{3}{\pi}$	$\frac{\sqrt{2}}{2\pi}\sqrt{9+4\sqrt{2}}$	$\frac{2}{\pi}$	$\frac{\sqrt{2}}{2\pi}\sqrt{9-4\sqrt{2}}$	$\frac{1}{\pi}$	$\frac{1}{12}$	$\frac{3}{4}\frac{8-5\sqrt{2}}{9+4\sqrt{2}}$	$\frac{9}{8}$	$\frac{3}{4}\frac{8+5\sqrt{2}}{9-4\sqrt{2}}$	$\frac{9}{4}$
2	a_2	0	$\mp\frac{1}{2\pi}$	0	$\pm\frac{1}{2\pi}$	0	$\frac{3}{\pi}$	$\frac{2}{\pi}$	$\frac{1}{\pi}$	$\frac{2}{\pi}$	$\frac{3}{\pi}$	$\frac{1}{12}$	$\frac{3}{8}(3-2\sqrt{2})$	$\frac{9}{4}$	$\frac{3}{8}(3+2\sqrt{2})$	$\frac{9}{12}$
1	a_3	0	$\pm\frac{\sqrt{2}}{2\pi}$	$\mp\frac{1}{\pi}$	$\pm\frac{\sqrt{2}}{2\pi}$	0	0	$\frac{\sqrt{2}}{\pi}\sqrt{3+2\sqrt{2}}$	$\frac{2}{\pi}$	$\frac{\sqrt{2}}{\pi}\sqrt{3-2\sqrt{2}}$	$\frac{4}{\pi}$	—	$\frac{3}{8}\frac{2-\sqrt{2}}{3+2\sqrt{2}}$	$\frac{9}{8}$	$\frac{3}{8}\frac{2+\sqrt{2}}{3-2\sqrt{2}}$	$\frac{9}{16}$
5	a_4	0	$\pm\frac{\sqrt{2}}{4\pi}$	$\pm\frac{1}{2\pi}$	$\pm\frac{\sqrt{2}}{4\pi}$	0	$\frac{3}{\pi}$	$\frac{\sqrt{2}}{2\pi}\sqrt{9+4\sqrt{2}}$	$\frac{2}{\pi}$	$\frac{\sqrt{2}}{2\pi}\sqrt{9-4\sqrt{2}}$	$\frac{1}{\pi}$	$\frac{1}{12}$	$\frac{3}{4}\frac{8-5\sqrt{2}}{9+4\sqrt{2}}$	$\frac{9}{8}$	$\frac{3}{4}\frac{8+5\sqrt{2}}{9-4\sqrt{2}}$	$\frac{9}{4}$
6	a_5	0	$\pm\frac{1}{2\pi}$	0	$\mp\frac{1}{2\pi}$	0	$\frac{3}{\pi}$	$\frac{2}{\pi}$	$\frac{1}{\pi}$	$\frac{2}{\pi}$	$\frac{3}{\pi}$	$\frac{1}{12}$	$\frac{3}{8}(3-2\sqrt{2})$	$\frac{9}{4}$	$\frac{3}{8}(3+2\sqrt{2})$	$\frac{9}{12}$
7	a_6	0	$\mp\frac{\sqrt{2}}{2\pi}$	$\pm\frac{1}{\pi}$	$\mp\frac{\sqrt{2}}{2\pi}$	0	0	$\frac{\sqrt{2}}{\pi}\sqrt{3+2\sqrt{2}}$	$\frac{2}{\pi}$	$\frac{\sqrt{2}}{\pi}\sqrt{3-2\sqrt{2}}$	$\frac{4}{\pi}$	—	$\frac{3}{8}\frac{2-\sqrt{2}}{3+2\sqrt{2}}$	$\frac{9}{8}$	$\frac{3}{8}\frac{2+\sqrt{2}}{3-2\sqrt{2}}$	$\frac{9}{16}$
8	a_7	0	0	0	0	0	$\frac{3}{\pi}$	$\frac{1}{\pi}$	$\frac{3}{\pi}$	$\frac{1}{\pi}$	$\frac{3}{\pi}$	$\frac{1}{12}$	$\frac{3}{4}(3-2\sqrt{2})$	$\frac{9}{12}$	$\frac{3}{4}(3+2\sqrt{2})$	$\frac{9}{12}$
9	a_8	0	$\mp\frac{\sqrt{2}}{4\pi}$	$\pm\frac{1}{2\pi}$	$\mp\frac{\sqrt{2}}{4\pi}$	0	$\frac{3}{\pi}$	$\frac{\sqrt{2}}{2\pi}\sqrt{9-4\sqrt{2}}$	$\frac{2}{\pi}$	$\frac{\sqrt{2}}{2\pi}\sqrt{9+4\sqrt{2}}$	$\frac{1}{\pi}$	$\frac{1}{12}$	$\frac{3}{4}\frac{16-11\sqrt{2}}{9-4\sqrt{2}}$	$\frac{9}{8}$	$\frac{3}{4}\frac{16+11\sqrt{2}}{9+4\sqrt{2}}$	$\frac{9}{4}$
31	a_9	0	0	0	0	0	$\frac{6}{\pi}$	$\frac{2}{\pi}$	$\frac{6}{\pi}$	$\frac{2}{\pi}$	$\frac{6}{\pi}$	$\frac{1}{24}$	$\frac{3}{8}(3-2\sqrt{2})$	$\frac{9}{24}$	$\frac{3}{8}(3+2\sqrt{2})$	$\frac{9}{24}$
32	a_{10}	0	$\mp\frac{\sqrt{2}}{2\pi}$	$\pm\frac{1}{\pi}$	$\mp\frac{\sqrt{2}}{2\pi}$	0	$\frac{6}{\pi}$	$\frac{\sqrt{2}}{\pi}\sqrt{9-4\sqrt{2}}$	$\frac{4}{\pi}$	$\frac{\sqrt{2}}{\pi}\sqrt{9+4\sqrt{2}}$	$\frac{2}{\pi}$	$\frac{1}{24}$	$\frac{3}{8}\frac{16-11\sqrt{2}}{9-4\sqrt{2}}$	$\frac{9}{16}$	$\frac{3}{8}\frac{16+11\sqrt{2}}{9+4\sqrt{2}}$	$\frac{9}{8}$
33	a_{11}	0	$\pm\frac{1}{\pi}$	0	$\mp\frac{1}{\pi}$	0	0	$\frac{2}{\pi}$	$\frac{4}{\pi}$	$\frac{2}{\pi}$	0	—	$\frac{3}{8}(3-2\sqrt{2})$	$\frac{9}{16}$	$\frac{3}{8}(3+2\sqrt{2})$	—
51	a_{12}	0	$\mp\frac{1}{\pi}$	0	$\pm\frac{1}{\pi}$	0	$\frac{6}{\pi}$	$\frac{4}{\pi}$	$\frac{2}{\pi}$	$\frac{4}{\pi}$	$\frac{6}{\pi}$	$\frac{1}{24}$	$\frac{3}{16}(3-2\sqrt{2})$	$\frac{9}{8}$	$\frac{3}{16}(3+2\sqrt{2})$	$\frac{9}{24}$
52	a_{13}	0	$\pm\frac{\sqrt{2}}{\pi}$	$\pm\frac{2}{\pi}$	$\pm\frac{\sqrt{2}}{\pi}$	0	0	$\frac{2\sqrt{2}}{\pi}\sqrt{3-2\sqrt{2}}$	$\frac{4}{\pi}$	$\frac{2\sqrt{2}}{\pi}\sqrt{3+2\sqrt{2}}$	$\frac{8}{\pi}$	—	$\frac{3}{16}\frac{10-7\sqrt{2}}{9-2\sqrt{2}}$	$\frac{9}{16}$	$\frac{3}{16}\frac{10+7\sqrt{2}}{3+2\sqrt{2}}$	$\frac{9}{32}$
53	a_{14}	0	0	0	0	0	$\frac{6}{\pi}$	$\frac{6}{\pi}$	$\frac{6}{\pi}$	$\frac{6}{\pi}$	$\frac{6}{\pi}$	$\frac{1}{24}$	$\frac{1}{8}(3-2\sqrt{2})$	$\frac{9}{24}$	$\frac{1}{8}(3+2\sqrt{2})$	$\frac{9}{24}$
21	a_{15}	0	$\pm\frac{\sqrt{2}}{2\pi}$	$\mp\frac{1}{\pi}$	$\pm\frac{\sqrt{2}}{2\pi}$	0	$\frac{6}{\pi}$	$\frac{\sqrt{2}}{\pi}\sqrt{9-4\sqrt{2}}$	$\frac{4}{\pi}$	$\frac{\sqrt{2}}{\pi}\sqrt{9+4\sqrt{2}}$	$\frac{2}{\pi}$	$\frac{1}{24}$	$\frac{3}{8}\frac{16-11\sqrt{2}}{9-4\sqrt{2}}$	$\frac{9}{16}$	$\frac{3}{8}\frac{16+11\sqrt{2}}{9+4\sqrt{2}}$	$\frac{9}{8}$
22	a_{16}	0	0	0	0	0	0	$\frac{4}{\pi}$	0	$\frac{4}{\pi}$	0	—	$\frac{3}{16}(3-2\sqrt{2})$	—	$\frac{3}{16}(3+2\sqrt{2})$	—
11	a_{17}	0	$\mp\frac{1}{\pi}$	0	$\pm\frac{1}{\pi}$	0	0	$\frac{2}{\pi}$	$\frac{4}{\pi}$	$\frac{2}{\pi}$	0	—	$\frac{3}{8}(3-2\sqrt{2})$	$\frac{9}{16}$	$\frac{3}{8}(3+2\sqrt{2})$	—
111	a_{18}	0	$\pm\frac{\sqrt{2}}{2\pi}$	$\pm\frac{1}{\pi}$	$\pm\frac{\sqrt{2}}{2\pi}$	0	0	$\frac{\sqrt{2}}{\pi}\sqrt{3-2\sqrt{2}}$	$\frac{2}{\pi}$	$\frac{\sqrt{2}}{\pi}\sqrt{3+2\sqrt{2}}$	$\frac{4}{\pi}$	—	$\frac{3}{8}\frac{10-7\sqrt{2}}{3-2\sqrt{2}}$	$\frac{9}{8}$	$\frac{3}{8}\frac{10+7\sqrt{2}}{3+2\sqrt{2}}$	$\frac{9}{16}$
211	a_{19}	0	0	0	0	0	$\frac{6}{\pi}$	$\frac{6}{\pi}$	$\frac{6}{\pi}$	$\frac{6}{\pi}$	$\frac{6}{\pi}$	$\frac{1}{24}$	$\frac{1}{8}(3-2\sqrt{2})$	$\frac{9}{24}$	$\frac{1}{8}(3+2\sqrt{2})$	$\frac{9}{24}$
212	a_{20}	0	$\pm\frac{\sqrt{2}}{4\pi}$	$\pm\frac{1}{2\pi}$	$\pm\frac{\sqrt{2}}{4\pi}$	0	$\frac{3}{\pi}$	$\frac{\sqrt{2}}{2\pi}\sqrt{9+4\sqrt{2}}$	$\frac{2}{\pi}$	$\frac{\sqrt{2}}{2\pi}\sqrt{9-4\sqrt{2}}$	$\frac{1}{\pi}$	$\frac{1}{12}$	$\frac{3}{4}\frac{8-5\sqrt{2}}{9+4\sqrt{2}}$	$\frac{9}{8}$	$\frac{3}{4}\frac{8+5\sqrt{2}}{9-4\sqrt{2}}$	$\frac{9}{4}$
311	a_{21}	0	$\pm\frac{\sqrt{2}}{2\pi}$	$\pm\frac{1}{\pi}$	$\pm\frac{\sqrt{2}}{2\pi}$	0	$\frac{6}{\pi}$	$\frac{\sqrt{2}}{\pi}\sqrt{9+4\sqrt{2}}$	$\frac{4}{\pi}$	$\frac{\sqrt{2}}{\pi}\sqrt{9-4\sqrt{2}}$	$\frac{2}{\pi}$	$\frac{1}{24}$	$\frac{3}{8}\frac{8-5\sqrt{2}}{9+4\sqrt{2}}$	$\frac{9}{16}$	$\frac{3}{8}\frac{8+5\sqrt{2}}{9-4\sqrt{2}}$	$\frac{9}{8}$
313	a_{22}	0	$\pm\frac{\sqrt{2}}{4\pi}$	$\mp\frac{1}{2\pi}$	$\pm\frac{\sqrt{2}}{4\pi}$	0	$\frac{3}{\pi}$	$\frac{\sqrt{2}}{2\pi}\sqrt{9-4\sqrt{2}}$	$\frac{2}{\pi}$	$\frac{\sqrt{2}}{2\pi}\sqrt{9+4\sqrt{2}}$	$\frac{1}{\pi}$	$\frac{1}{12}$	$\frac{3}{4}\frac{16-11\sqrt{2}}{9-4\sqrt{2}}$	$\frac{9}{8}$	$\frac{3}{4}\frac{16+11\sqrt{2}}{9+4\sqrt{2}}$	$\frac{9}{4}$
312	a_{23}	0	$\mp\frac{2}{\pi}$	0	$\pm\frac{2}{\pi}$	0	0	$\frac{4}{\pi}$	$\frac{8}{\pi}$	$\frac{4}{\pi}$	0	—	$\frac{3}{16}(3-2\sqrt{2})$	$\frac{9}{32}$	$\frac{3}{16}(3+2\sqrt{2})$	—

where

$$D_0 = (1+a_7^2+\ \dots\ +a_0^2),\quad D_1 = 2(a_7+a_7a_6+\ \dots\ +a_1a_0),\ \dots,\quad D_7 = 2(a_1+a_7a_0),$$

$$D_8 = 2a_0 \quad \text{and} \quad N_0 = a_7J(1)+a_6[J(2)+a_7J(1)]+a_5[J(3)+a_7J(2)+a_6J(1)]+\ \dots$$

$$+a_1[J(7)+a_7J(6)+\ \dots\ +a_2J(1)]-a_0^2,\quad N_1 = a_6J(1)+a_5[J(2)+a_7J(1)]+\ \dots$$

$$+a_0[J(7)+a_7J(6)+\ \dots\ +a_2J(1)]+J(1)+a_7[J(2)+a_7J(1)]+\ \dots$$

$$+a_2[J(7)+a_7J(6)+\ \dots\ +a_2J(1)]-a_1a_0, \dots, \quad N_6 = a_1J(1)+a_0[J(2)+a_7J(1)]$$
$$+[J(6)+a_7J(5)+\ \dots\ +a_3J(1)]+a_7[J(7)+a_7J(6)+\ \dots\ +a_2J(1)]-a_6a_0,$$
$$N_7 = a_0J(1)+[J(7)+a_7J(6)+\ \dots\ +a_2J(1)]-a_7a_0, \quad N_8 = -a_0,$$

a_i are coefficients of a characteristic equation expressed by α_i in point (6) and *J(m)* are boundary conditions expressed by α_i in point (7).

Following expressions (9), (11) and (15) of the previous paper (Michalski et al. (1980)) the peak shifts $\Delta h_3,(h_3),$ peak broadening $\Delta w(h_3)$ and changes of the peak maxima intensity $I_{max}(h_3)$ have the form

$$\Delta h_3(h_3) = \tfrac{1}{32} \sum_{m=0}^{8} mD_m \sin\left(\frac{m\pi}{4} h_3\right), \tag{31}$$

$$I_{max}(h_3) = \frac{2\sum_{m=0}^{8} N_m \cos\left(\frac{m\pi}{4} h_3\right)}{\sum_{m=0}^{8} D_m \left[\cos\left(\frac{m\pi}{4} h_3\right) - \frac{m\pi}{4}\Delta h_3 \sin\left(\frac{m\pi}{4} h_3\right) - \left(\frac{m\pi}{4}\Delta h_3\right)^2 \frac{1}{2}\cos\left(\frac{m\pi}{4} h_3\right)\right]}, \tag{33}$$

$$w(h_3) = \frac{1}{\pi}\sqrt{\sum_{m=0}^{8} D_m \left[\cos\left(\frac{m\pi}{4} h_3\right) - \frac{m\pi}{4}\Delta h_3 \sin\left(\frac{m\pi}{4} h_3\right) - \left(\frac{m\pi}{4}\Delta h_3\right)^2 \frac{1}{2}\cos\left(\frac{m\pi}{4} h_3\right)\right]}, \tag{32}$$

where h_3 = 8M, 8M± 1, ±2, ±3, ±4. The results of calculations are presented in Table II.

9. *Analysis of stacking faults in the 8H(44) crystals*

Table II presents 16 equations with experimentally determined values of $\Delta h_3(h_3)$, $\Delta w(h_3)$ and $I_{max}(h_3)$ for different single crystal reflexions (h_3 = 8M, 8M± 1, ±2, ±3, ±4). There are 23 unknown α_i probabilities of the occurrence of particular types of faults. Thus, it is not possible to determine the probabilities α_i for the examined structure by the solution of a general system of equations. One can find the. expressions for two more experimentally observable parameters from peak asymmetry measurements. Changes in the integrated intensity can be used as a measure of faulting instead of changes in the peak maxima. However, (following Pandey and Krishna (1976)) the peak asymmetry and changes in integrated intensities are usually too small to be estimated experimentally with sufficient accuracy. Thus, peak shifts and the half width seem to be the best measures of faulting. The initial elimination of some type of faults based on the consideration of the energy of SFE-stacking faults proposed by Pandey and Krishna (1976) for the structure 6H(33) is also impossible for the 8H(44) structure. There is no basis to justify the assumptions, based on the statistics of the examined structures, about the probabilities of the occurrence of some types of faults.

It can be seen (see Table II) that the information about the type of faults occurring in crystals is contained in the presence or absence of peak shifts $\Delta h_3(h_3)$ for different reflexions and in the sign of the peak shifts. On this basis all the possible diffraction patterns can be divided into 13 essential types (obtained as on effect of different combinations of the above parameters) differing from each other by qualitative features. For six of them we can assign the single types of fault (22), (33), (1), (7,) (6) and (3) and for the remaining we can assign the group of non distinguishable faults (11)-(312), (52)-(111), (8)--(31)

TABLE III

The essential diffraction patterns from 8H(44) structures with stacking faults

Description of the diffraction pattern					Zhdanov's symbols of faults
$\Delta W\ (h_3)$	$\Delta h_3\ (h_3)$	sign of $\Delta h_3(h_3)$ for h_3 equal to			
		$8M\pm1$	$8M\pm2$	$8M\pm3$	
$\Delta W(8M,8M\pm2,\pm4)=0$ $\Delta W(8M\pm1\pm3)\neq0$	$\Delta h_3(8M,8M\pm1,\pm2,\pm3,\pm4)=0$	0	0	0	(22)
$\Delta W(8M,8M\pm4)=0$	$\Delta h_3(8M,8M\pm2,\pm4)=0$	$\pm$	0	$\mp$	(33)
$\Delta W(8M\pm1,\pm2,\pm3)\neq0$	$\Delta h_3(8M\pm1,\pm3)\neq0$	$\mp$	0	$\pm$	(11), (312)
$\Delta W(8M)=0$	$\Delta h_3(8M,8M\pm4)=0$	$\pm$	$\mp$	$\pm$	(1)
$\Delta W(8M\pm1,\pm2,\pm3,\pm4)\neq0$	$\Delta h_3(8M\pm1,\pm2,\pm3)\neq0$	$\mp$	$\pm$	$\mp$	(7)
		$\pm$	$\pm$	$\pm$	(52), (111)
$\Delta W(8M,8M\pm1,\pm2,\pm3,\pm4)\neq0$	$\Delta h_3(8M,8M\pm1,\pm2,\pm3,\pm4)=0$	0	0	0	(8),(31),(53),(211)
	$\Delta h_3(8M,8M\pm2,\pm4)=0$	$\pm$	0	$\mp$	(6)
	$\Delta h_3(8M\pm1,\pm3)\neq0$	$\mp$	0	$\pm$	(2), (51)
	$\Delta h_3(8M,8M\pm4)=0$	$\mp$	$\mp$	$\mp$	(3)
	$\Delta h_3(8M\pm1,\pm2,\pm3)\neq0$	$\mp$	$\pm$	$\mp$	(9),(32)
		$\pm$	$\mp$	$\pm$	(21),(313)
		$\pm$	$\pm$	$\pm$	(5),(212),(311)

~(53)-(211), (2)-(51), (9)-(32), (21)-(313) and (5)-(212)-(311). The description of the main diffraction patterns is presented in Table III.

If X-ray diffraction photographs of the examined crystals are exactly adequate to one of the 13 main diffraction patterns from Table III, the analysis of the faults in these crystals is simple. To estimate α_i probabilities it is sufficient to measure one of the parameters $\Delta w(h_3)$, $\Delta h_3(h_3)$ or $I_{max}(h_3)$ and to solve one of the 16 equations with one unknown α_i. It can be seen that for non distinguishable faults the relations $2\alpha_{17} = \alpha_{23}$, $\alpha_{13} = 2\alpha_{18}$, $\alpha_{12} = 2\alpha_2$ $\alpha_{10} = 2\alpha_8$, $\alpha_{15} = 2\alpha_{22}$, $\alpha_{21} = 2\alpha_{20} = 2\alpha_4$, $2\alpha_7 = \alpha_9 = \alpha_{14} = \alpha_{19}$ are valid. In the other cases it is necessary to settle down from which of 13 main diffraction patterns there are the characteristic features simultaneously observed on the X-ray diffraction photographs. We can get the estimation of α_i - probabilities by solving adequate numbers of equations.

Based on the above method the analysis of stacking faults in 8H(44) structures of ZnSe doping Mn and ZnS doping In crystals was made. Based on the qualitative characteristic features of X-ray diffraction photographs (Fig. 2) (the great peak broadening of reflexions with $h_3 = 8M\pm1, \pm3$, perishable peak broadening of reflexions with $h_3 = 8M$, $8M\pm2, \pm4$, absence of peak shifts for reflexions with $h_3 = 8M$, $8M\pm2, \pm4$ and sign ± of peak shifts for reflexions with $h_3 = 8M\pm1$ and (-1)± for $h_3 == 8M\pm3$) the occurrence of (22)-type faults principially and (33) and (6)-perishable type faults was found. The following parameters were measured

Sample	*a*	b	c	*d*	*e*	f	*g*
$\Delta w(h_3 = 2)$	0.05	0	0	0	0.05	0	0.05
$\Delta w(h_3 = 3)$	0.2	0.1	0.25	0.3	0.1	0.3	0.5
$\Delta w(h_3 = 4)$	0.05	0.05	0.05	0.05	0.05	0	0

3 equations are necessary

$$\Delta w(8M+2) = \frac{1}{\pi}\alpha_5 + \frac{4}{\pi}\alpha_{11},$$

$$\Delta w(8M+3) = \frac{2}{\pi}\alpha_5 + \frac{2}{\pi}\alpha_{11} + \frac{4}{\pi}\alpha_{16},$$

$$\Delta w(8M+4) = \frac{3}{\pi}\alpha_5.$$

Probabilities of α_i occurrence of particular types of faults are

Zdanov's Symbol of fault	Sample α_i	*a*	*b*	*c*	*d*	*e*	*f*	*g*
(6)	α_5	0.05	0.05	0.05	0.05	0.05	0	0
(33)	α_{11}	0.03	0	0	0	0.03	0	0.04
(22)	α_{16}	0.12	0.05	0.17	0.21	0.04	0.24	0.37

and hexagonalities of examined crystals

sample	*a*	*b*	*c*	*d*	*e*	*f*	*g*
a_h	0.28	0.26	0.29	0.20	0.26	0.30	0.35

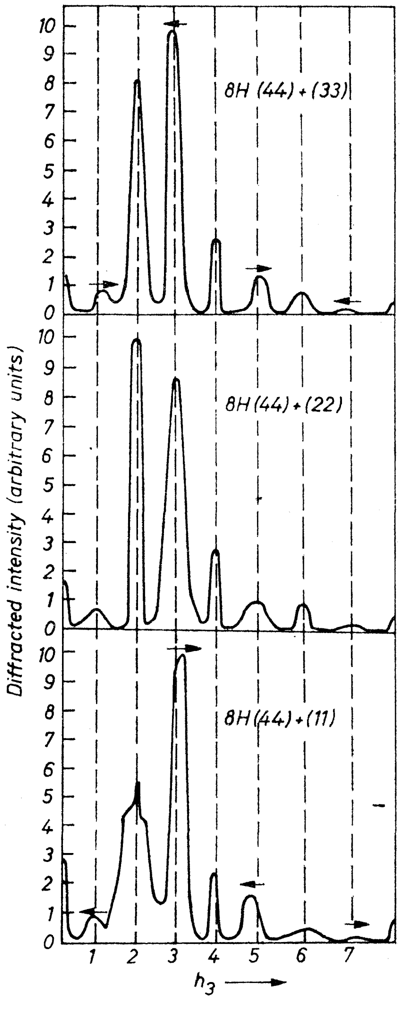


Fig. 3. The distribution of $I_{10.l}$ intensity obtained by model analysis

To illustrate the peak shifts $\Delta h_3(h_3)$, peak broadening $\Delta w(h_3)$ and change in the peak maxima intensity $I_{max}(h_3)$ and to compare them with the method of model analysis (Pałosz (1977)), the distribution of $I_{10.l}$ intensity obtained by model analysis is presented in Fig. 3.

10. Discussion

The complete characterization of all the possible X-ray diffraction patterns involving stacking faults in the 8H(44) structure was presented. Using the above method one can also similarly characterize 10H(55), 12H(66) and other *nH(n/2 n/2)* structures, which are most often met in $A^{II}B^{VI}$ compounds. In this method the information about the type of fault is reached with minimum of work. Such characteristics although qualitative, can often be useful for stacking faults. Moreover, the accuracy of quantitative evaluation of fault content depends on the accuracy of measuring of $\Delta h_3(h_3)$, $\Delta w(h_3)$ or $I_{max}(h_3)$ parameters. These last ones can be different depending on the actual necessity, the apparatus possibility and the time devoted to investigations. It is an important feature of our method with respect to others given e.g. in Pałosz (1977), Farhas-Jahnke (1973) and Kakinoki and Komura (1965).

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