Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.

Acta Cryst. (1969). A**25**, 385

An application of the Patterson method to the determination of layer sequences in polytypes with close-packed structures.

By J. Kakinoki, E. Kodera and T. Aikami, *Department of Physics, Faculty of Science, Osaka City University, Sugimoto-cho, Sumiyoshi-ku, Osaka, Japan*

(*Received* 20 *August* 1968 *and in revised form* 30 *August* 1968)

The Patterson method is applied to the determination of layer sequences in polytypes with close-packed structures and a Table is given which shows the relationship between the Zhdanov symbol and a set of quantities which are directly available from observed intensities.

In the determination of the layer sequence in close-packed structures, it is convenient to use the unitary intensities, I_l, defined as

$$I_l = \left| \sum_{p=0}^{P-1} \Delta_p \exp(ipl\theta) \right|^2$$

where P is the number of layers contained in one period and $\theta = 2\pi/P$. Corresponding to the cases in which the pth layer is $A(00)$, $B(\frac{2}{3}\ \frac{1}{3})$ or $C(\frac{1}{3}\ \frac{2}{3})$ in the hexagonal lattice,

$$\Delta_p = 1 \text{ for } A, \quad \varepsilon^* \text{ for } B \quad \text{and} \quad \varepsilon \text{ for } C$$

with

$$\varepsilon = \exp\{2\pi i(h-k)/3\}\,.$$

I_l can be transformed as

$$I_l^{(\pm)} = -(P^2/2)\delta_{l0} + (\tfrac{3}{2}) \sum_{m=0}^{P-1} N_m^0 \cos ml\theta \pm (\sqrt{3}/2) \sum_{m=0}^{P-1} D_m \sin ml\theta$$

with

$$D_m = N_m^+ - N_m^-\,,$$

where δ_{l0} is Kronecker's delta, N_m^0 is the number of pairs of two layers of the same kind separated by m layers, N_m^+ that of positive pairs ($A\cdots B$, $B\cdots C$ or $C\cdots A$), N_m^- that of negative pairs ($A\cdots C$, $C\cdots B$ or $B\cdots A$) and + and − in ± indicate respectively intensities along the plus and the minus lines for which $h-k=3n\pm1$.

By the use of the cosine and the sine transformations of $I_l^{(+)}$, N_m^0 and D_m are given by

$$N_m^0 = (2/3P)C_m + P/3$$
$$D_m = (2/\sqrt{3}P)S_m \equiv 3D_m^* \text{ (put)}$$

with

$$C_m = \sum_{l=0}^{P-1} I_l^{(+)} \cos ml\theta \quad \text{and} \quad S_m = \sum_{l=0}^{P-1} I_l^{(+)} \sin ml\theta\,,$$

where the summation with respect to l is carried out only along the plus line over one period from 0 to $P-1$ in reciprocal space. C_m and S_m are the Patterson functions in the case of the close-packed structures. D_m is shown to be integral multiples of 3 and we put $D_m = 3D_m^*$.

Table 1 shows the relation between the quantities N_m^0 and D_m^* and the Zhdanov symbol (Zhdanov, 1945) which is expressed as†

$$(a_1\,\bar{b}_1\,a_2\,\bar{b}_2\,\ldots\,a_k\,\bar{b}_k)$$

† In the original form, ¯ on each b_i is omitted.

where a_i and b_i mean respectively the numbers of successive positive and negative neighbours. m_1, $m_{\bar{1}}$, m_2, $m_{\bar{2}}$ ... *etc.* in Table 1 mean respectively the frequencies of letters 1, $\bar{1}$, 2, $\bar{2}$, ... *etc.* contained in the Zhdanov symbol and $m_{1\bar{1}}$, $m_{\bar{2}1}$, $m_{1\bar{2}1}$, ... *etc.* are those of sequences $1\bar{1}$, $\bar{2}1$, $1\bar{2}1$, ... *etc.* in the Zhdanov symbol. The conditions

$$C_0 = P^2, \quad C_1 = -P^2/2 \quad \text{and} \quad S_1 = -S_2$$

corresponding to $N_0^0 = P$, $N_1^0 = 0$ and $D_1^* = (a-b)/3 = -D_2^*$, respectively, are used for the determination of the scale factor when the observed intensities measured in an arbitrary unit are transformed into the unitary intensities.

In deriving the relations in Table 1, we use the relations

$$\sum_{\alpha=1}^{\alpha^*} m_\alpha = \sum_{\beta=1}^{\beta^*} m_{\bar{\beta}} = k\,, \quad \sum_{\alpha=1}^{\alpha^*} \alpha m_\alpha = a \quad \text{and} \quad \sum_{\beta=1}^{\beta^*} \beta m_{\bar{\beta}} = b\,,$$

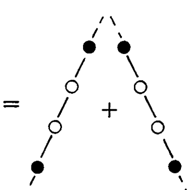
where α^* and β^* are respectively the maximum values of α and β in the Zhdanov symbol. a and b are defined as

$$a = \sum_{i=1}^{k} a_i \quad \text{and} \quad b = \sum_{i=1}^{k} b_i$$

and they give the basic partition $(a, \bar{b})$ with the degree of partition, k, in the Zhdanov symbol (Patterson & Kasper 1959). From these definitions, we have at once

$$a+b=P \quad \text{and} \quad a-b = \begin{cases} 6n & \text{for } P \text{ even} \\ 3+6n & \text{for } P \text{ odd.} \end{cases}$$

For example, the relation $N_3^0 = P - 4k + (m_1 + m_{\bar{1}})$ in Table 1 can be derived as follows:

$N_3^0 =$  $= \sum_{\alpha=3}^{\alpha^*} (\alpha-2)m_\alpha + \sum_{\beta=3}^{\beta^*} (\beta-2)m_{\bar{\beta}}$

$$= \sum_{\alpha=1}^{\alpha^*} \alpha m_\alpha - 2\sum_{\alpha=1}^{\alpha^*} m_\alpha + m_1 + \sum_{\beta=1}^{\beta^*} \beta m_{\bar{\beta}} - 2\sum_{\beta=1}^{\beta^*} m_{\bar{\beta}} + m_{\bar{1}}$$
$$= a - 2k + m_1 + b - 2k + m_{\bar{1}} = P - 4k + (m_1 + m_{\bar{1}})\,.$$

By the use of Table 1, the layer sequence can be uniquely determined for a smaller value of P. For a larger value of P,

Table 1. *Relations between Zhdanov symbol and* N^0_m *and* $D^*_m = D_m/3$

m	N^0_m	$D^*_m = D_m/3 = (N^+_m - N^-_m)/3$
0	P	0
1	0	$(a-b)/3$
2	$2k$	$-(a-b)/3$
3	$P-4k+(m_1+m_{\bar{1}})$	$-(m_1-m_{\bar{1}})$
4	$2k-2(m_1+m_{\bar{1}})$ $+(m_2+m_{\bar{2}})+2(m_{1\bar{1}}+m_{\bar{1}1})$	$(a-b)/3+2(m_1-m_{\bar{1}})$ $+(m_2-m_{\bar{2}})$
5	$4k+(m_1+m_{\bar{1}})$ $-2(m_2+m_{\bar{2}})-4(m_{1\bar{1}}+m_{\bar{1}1})$ $-2(m_3+m_{\bar{3}})-(m_{2\bar{1}}+m_{\bar{2}1}+m_{1\bar{2}}+m_{\bar{1}2})$ $+(m_{1\bar{1}1}+m_{\bar{1}1\bar{1}})$	$-(a-b)/3-(m_1-m_{\bar{1}})$ $-2(m_2-m_{\bar{2}})$ $+(m_{2\bar{1}}-m_{\bar{2}1}-m_{1\bar{2}}+m_{\bar{1}2})-(m_{1\bar{1}1}-m_{\bar{1}1\bar{1}})$
6	$P-8k+2(m_1+m_{\bar{1}})$ $+(m_2+m_{\bar{2}})+2(m_{1\bar{1}}+m_{\bar{1}1})$ $+4(m_3+m_{\bar{3}})+2(m_{2\bar{1}}+m_{\bar{2}1}+m_{1\bar{2}}+m_{\bar{1}2})$ $-2(m_{1\bar{1}1}+m_{\bar{1}1\bar{1}})$ $+(m_4+m_{\bar{4}})-(m_{3\bar{1}}+m_{\bar{3}1}+m_{1\bar{3}}+m_{\bar{1}3})$ $+2(m_{2\bar{2}}+m_{\bar{2}2})+(m_{2\bar{1}1}+m_{\bar{2}1\bar{1}}+m_{1\bar{1}2}+m_{\bar{1}1\bar{2}})$ $-2(m_{1\bar{2}1}+m_{\bar{1}2\bar{1}})+2(m_{1\bar{1}1\bar{1}}+m_{\bar{1}1\bar{1}1})$	$-2(m_1-m_{\bar{1}})$ $+(m_2-m_{\bar{2}})$ $-2(m_{2\bar{1}}-m_{\bar{2}1}-m_{1\bar{2}}+m_{\bar{1}2})+2(m_{1\bar{1}1}-m_{\bar{1}1\bar{1}})$ $-(m_4-m_{\bar{4}})-(m_{3\bar{1}}-m_{\bar{3}1}-m_{1\bar{3}}+m_{\bar{1}3})$ $+(m_{2\bar{1}1}-m_{\bar{2}1\bar{1}}+m_{1\bar{1}2}-m_{\bar{1}1\bar{2}})$

$m \geq 7$ are omitted to save space.

the number of models to be examined is limited to a very small number in spite of a tremendous number of independent structures for a given P, for example, about 10^7 independent structures for $P=34$. Some new structures of ZnS such as

$$(7\ \bar{7})\dagger,\ (8\ \bar{6})_3,\ (9\ \bar{5})_3 \quad \text{and} \quad (11\ \bar{3})_3$$

can be determined by applying the present method.

† The structure (7 $\bar{7}$) was recently reported by Steinberger, Mardix & Brafman (1967).

Other important relations and details will be reported in the near future.

References

PATTERSON, A. L. & KASPER, J. S. (1959). *International Tables for X-Ray Crystallography*, Vol. II, p. 344. Birmingham: Kynoch Press.

STEINBERGER, I. T., MARDIX, S. & BRAFMAN, O. (1967). *Acta Cryst.* **22**, 805.

ZHDANOV, G. S. (1945). *C. r. Acad. Sci. URSS*, **48**, 43.