nichts anderes darstellen als örtlich begrenzte Kristallbereiche mit der α-Sm-bzw. der *ABCACB*-Struktur.

Auch bei den Fehlern höherer Ordnung [Fig. 3, Kurvenzug (2) usw.] ist die Symmetrie der Darstellung klar erkennbar. Ferner stellen natürlich auch hier wieder die Kurvenzüge der Stapelfehler Kurvenzüge von Idealstrukturen dar.

6. Simulation von Kristallen mit Stapelfehlern durch Analog-Stromkreise

Die entwickelte Symbolik ist geeignet, Kristalle mit Stapelfehlern durch elektrische Stromkreise zu simulieren. Betrachten wir einen realen Kristall mit Stapelfehlern, so durchläuft z.B. im Wegdiagramm der Fig. 2 ein Aufpunkt einen bestimmten Weg, wenn wir von der ersten zur letzten Netzebene vorwärtsschreiten. Dieser Weg ist durch die Art der Struktur und die Häufigkeit der einzelnen Stapelfehlertypen charakterisiert.

Denken wir uns nun dieses Wegdiagramm als elektrisches Leitungsdiagramm und den Aufpunkt als elektrischen Impuls, so können wir, wenn wir an den 'Weichen' statistische 'Gates' anbringen, den Aufbau des Kristalls simulieren. Weichen existieren im Wegdiagramm der Fig. 2 in den untersten Punkten des linken und mittleren Kreises, wie auch in den obersten Punkten des mittleren und rechten Kreises. Die statistischen Gates sind so eingestellt, dass mit einer bestimmten Wahrscheinlichkeit w_i ($i=1, 2, 3$ u. 4) der gerade Weg und mit der Wahrscheinlichkeit $1-w_i$ der krumme Weg eingeschlagen wird.

Für die tatsächliche Realisierung eines solchen Stromkreises ist es erstens notwendig, an bestimmten Stellen des Kreises für eine Abnahme eines Signals für die Steuerung eines Computerprogramms Vorsorge zu tragen. Zweitens sind Verzögerungsleitungen einzubauen, damit die abgenommenen Signale getrennt registriert werden können. Ferner ist dann drittens noch an der am meisten durchlaufenen Stelle des Kreises für eine Verstärkung bzw. Wiedererzeugung des Impulses zu sorgen.

Mit einem solchen Analog-Stromkreis ist es z.B. möglich, die Streuung von Röntgenstrahlen an einem beliebigen Kristall mit statistisch verteilten Stapelfehlern zu behandeln und die Intensitätsverteilung im k-Raum zu berechnen. Falls durch weitere Gate-Kreise für eine statistische Änderung der Grössen w_i gesorgt wird, können die Effekte einer nicht statistischen Anordnung von Stapelfehlern studiert werden.

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The Polytypic Growth in Zinc Sulphide Crystals

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Various mechanisms for the polytypic growth in zinc sulphide crystals have been discussed. It has been pointed out that the polytypic growth in this compound is a result of the ordering of f.c.c. microtwins along the ⟨111⟩ directions. A comparison between the structures actually found and those expected from consideration of the periodically repeated f.c.c. type microtwins shows a good agreement. The periodic occurrence of f.c.c. type microtwins has been shown to result from $2H$ structures containing growth faults only, when faults due to slip at alternate layers and axial screw dislocations operate simultaneously. This mechanism is assumed to operate only at a stage when crystals are growing, and it can successfully predict almost all structures which are actually found in ZnS polytypes. Only a few polytypes (three, $9R$, $12R$, and $21R$, out of more than a hundred) with structures not fitting the above mechanism have been attributed to the insertion of periodic stacking faults in some other polytypes (which are generated in accordance with the proposed mechanism) at a later stage of the crystal growth.

Introduction

Polytypic growth is a phenomenon, characterized by the periodic repetition of stacking faults in close-packed planes of solids, leading to a series of new structures which are identical in the **a** and **b** directions and differ only in the **c** direction (perpendicular to the stacking of layers) of the unit cell. Each member of such a structure series is known as a polytype. Like SiC, PbI_2, CdI_2 and many other compounds, ZnS exhibits polytypic growth. The growth process of polytypes has been a subject of discussion for many years. Numerous theories have so far been proposed but none of them seems to give a complete explanation. The screw dislocation mechanism, which was proposed by Frank (1951, 1952) for SiC polytypes and was developed further by Mitchell (1957) and Krishna & Verma (1965), cannot, as such, be applicable to ZnS polytypes. This is first because the stable phase (at the temperature at which ZnS polytypes are synthesized) is 2*H*, from which screw dislocations cannot produce polytypes (Mitchell, 1959), and secondly because the ZnS polytypes do not contain those basic units like 33, 32, 11, 22 *etc.* in the Zhdanov symbol (Zhdanov & Minervina, 1946) which have been found in SiC and CdI_2 polytypes. Mardix, Kalman & Steinberger (1968) proposed the mechanism of the periodic slip process but they did not mention the cause of periodic slips, and furthermore its efficiency is limited only to transforming one polytype to another. Daniels (1966) proposed that a suitably compounded system of axial (perfect or partial) and partial dislocations in the (0001) plane of 2*H* will produce polytypes. His proposal, however, has a drawback in that it introduces an increasing number of (11) structure units in the Zhdanov symbol of polytypes with an increasing number of layers in their unit cell. This model will also be inefficient in producing many kinds of polytypes *e.g.* 9*R*, 15*R*, 21*R*, 4*H*, 8*H*, 10*H*, 16*H*, 20*H*, 24*H*, 28*H etc.*

More than a hundred ZnS polytypes with known crystal structures have so far been reported and there seems no upper limit on the number of polytypes. All these polytypes, except a few (9*R*, 12*R* and 21*R*), show the three following structural characteristics:

(1) The (11) units in the Zhdanov symbol are absent.

(2) All the possible numbers like 2, 3, 4, 5, 6, 7, ..., 35, ... *etc.* in the Zhdanov notation are found to appear.

(3) The polytypes contain most of the layers in the f.c.c. arrangement such that the percentage, *p*, of this type of layer is always ≥50%.

Almost all the polytypes have been grown above 1020°C. Thus any mechanism involving dislocations must start from 2*H* and the resulting structures should show the characteristics as mentioned above. Unfortunately none of the existing theories can explain the origin of these characteristics. The purpose of this paper is therefore to present a possible mechanism which can produce polytypes during the growth of ZnS crystals.

Possible polytypic structures from f.c.c. microtwins

The structural characteristics (2) and (3) indicate that a large number of 3*C* type units arranged in proper sequence are present in ZnS polytypes. These type of structures therefore are expected to be derived from the f.c.c. type of microtwins which repeat periodically in the ⟨111⟩ directions. The relations between twins of an order of unit cells (referred to as microtwins in this paper) and polymorphs or polytypes have been discussed by Ito (1950) and by Sadanaga & Takeuchi (1961), but here the aforesaid structural properties of ZnS polytypes are deduced as follows.

Let a system of 180° rotational microtwins with n_1 layers in the $(A \rightarrow B \rightarrow C \rightarrow A \ldots)$ stacking sequence and n_2 layers in the $(A \rightarrow C \rightarrow B \rightarrow A \ldots)$ stacking sequence repeat periodically along the ⟨111⟩ directions of a f.c.c. structure. Depending upon whether $n_1 - n_2 = 3n$ or not (*i.e.* the first and last layers of the combined twin system are in different or in the same orientation), the polytypes of the type *NH* or 3*NR* with $N = n_1 + n_2$ will be formed. Every layer (*A*, *B* or *C*) in this notation represents a ZnS double layer and the sense of the Zn → S vector remains in the same direction throughout the structure. The Zhdanov notation of these polytypes can then be written as (n_1n_2) or $(n_1n_2)_3$. As a f.c.c. structure or its twin can only be imagined when it has at least three layers (*ABC* or *ACB*) in the close packed assembly, the lowest value of n_1 or n_2 (*i.e.* the average number of layers in each twin block) can be shown not to fall below 2. For example in the 10*H* polytypes with stacking sequence $AB\underline{C}BACBACBA$ ..., the $\underline{C}$ layer is common in both the sequences (*i.e.* $AB\underline{C}$ and $\underline{C}BACBACBA$ ...). Although $AB\underline{C}$ is in the sequence of a f.c.c. structure, the value of n_1 is 2 and that of n_2 is 8. Thus in general the values of n_1 and n_2 will subject to

$$n_1, n_2 = 3n' \quad \text{or} \quad 3n' \pm 1 \tag{1}$$

where n' is an integer ≥1.

It appears from equation (1) that all the numbers except 1 can appear in the Zhdanov symbol of polytypes in the f.c.c. twin representation.

In every assembly of twins, each twin block (*i.e.* each block in 180° rotational twin orientation to the other) contains one layer in the h.c.p. stacking sequence. For example, in 6*H* with stacking sequence $ABC\underline{A}CB\underline{A}$ ... which contains two twin blocks ($ABC\underline{A}$ and $\underline{A}CB\underline{A}$), the underlined layers $\underline{A}_s$ are in the h.c.p. stacking sequence. If an *N*-layered polytype contains n_T twin blocks, then the percentage, *p*, of layers with f.c.c. stacking sequence can be written as

$$p = [1 - n_T/N] \times 100 \tag{2}$$

where $2 \leq n_T \leq N/2$.

The limiting value of n_T has been imposed from polytypic structures. Taking minimum and maximum values of n_T as 2 and $N/2$, respectively, it is easy to see that all possible values of *p* will lie between 50 and 100.

From Table 1, one can see that the results based on periodically repeated f.c.c. type twins along the ⟨111⟩ direction are in agreement with the observed structure of polytypes and thus it is expected that a mechanism which can generate such a type of twins should operate in 2*H* type crystals.

Table 1. ZnS *polytypes*

Sample No.	Ramsdell notation	Zhdanov notation	% layer in f.c.c. orientation
1	4*H*	(22)	50·0
2	6*H*	(33)	66·6
3	8*H*	(44)	75·0
4	9*R*	$(21)_3$	33·3
5	10*H*	(55)	80·0
6	10*H*	(82)	80·0
7	12*R*	$(31)_3$	50·0
8	14*H*	(77)	85·7
9	14*H*	(5423)	71·5
10	15*R*	$(32)_3$	60·0
11	16*H*	(88)	87·5
12	18*R*	$(42)_3$	66·0
13	20*H*	(533423)	70·0
14	20*H*	(522362)	70·0
15	21*R*	$(3112)_3$	42·8
16	24*H*	(7557)	83·3
17	24*H*	(9564)	83·3
18	24*H*	(16422)	83·3
19	24*H*	(71052)	83·3
20	24*H*	(8943)	83·3
21	24*H*	(33242253)	66·6
22	24*H*	(33422433)	66·6
23	24*H*	(159)	91·6
24	24*R*	$(53)_3$	75·0
25	26*H*	(17423)	84·6
26	28*H*	(9559)	85·7
27	36*R*	$(6222)_3$	66·6
28	48*R*	$(97)_3$	87·5
29	48*R*	$(124)_3$	87·5
30	48*R*	$(7423)_3$	75·0
31	48*R*	$(433222)_3$	62·5
32	60*R*	$(182)_3$	90·0
33	60*R*	$(11432)_3$	80·0
34	60*R*	$(522353)_3$	70·0
35	72*R*	$(61152)_3$	83·3
36	72*R*	$(9546)_3$	83·3

Note: Remaining ZnS polytypes follow the same trend and those are not listed here.

Generation mechanism of periodic f.c.c. microtwins

Normally the crystals of ZnS showing polytypic growth have been synthesized from the vapour phase above the temperature of the 3*C* to 2*H* phase transformation. At this temperature only the 2*H* phase is expected to be stable. Thus to explain the origin of periodic microtwins (the polytypic growth) the following assumptions are made:

(i) At an elevated temperature (> 1020 °C) the ZnS crystals of the 2*H* type start growing. The stacking faults are introduced during the growth.

(ii) Either because of the temperature inhomogeneity or the presence of trace impurities, which may change the conditions of phase stability, complex mechanical stresses are set up in the crystal flake. These stresses in turn result in slips at alternate layers and axial screw-dislocations (*i.e.* along the [0001] axis) in the 2*H* crystal containing growth faults only.

This causes polytypes to generate during the growth process of crystals. Slips at alternate layers cause 2*H* crystals to transform into a 3*C* structure (Blank, Delavignette & Amelinckx, 1962). However, when the crystals contain growth faults, this process produces a 3*C* structure on either side of the faults in 180° rotational twin orientation, *e.g.*

$$\begin{array}{r}
h\ h\ h\ h\ h\ k\ h\ h\ h\ h\ h\ h \\
A\ B\ A\ B\ A\ \overline{\underline{B}}\ C\ B\ C\ B\ C\ B \\
\downarrow\qquad\qquad\qquad\qquad\qquad\quad \\
C\ A\ C\ A\ B\ A\ B\ A\ B\ A \\
\downarrow\qquad\qquad\qquad\qquad \\
B\ C\ A\ C\ A\ C\ A\ C \\
\downarrow\qquad\qquad\quad \\
B\ A\ B\ A\ B\ A \\
\downarrow\qquad\quad \\
C\ B\ C\ B \\
\downarrow\quad \\
A\ C \\
k\ k\ k\ k\ k\ \underline{h}\ k\ k\ k\ k\ k\ k
\end{array}$$

or

$$A\ B\ C\ A\ B\ \underline{C}\ B\ A\ C\ B\ A\ C$$

Here in the (*hk*) notation *h* denotes the layer in h.c.p. orientation and *k* denotes the layers in f.c.c. orientation.

When an axial screw-dislocation operates simultaneously with slip at alternate layers, it produces a growth step, which consists of a f.c.c. twin structure, on the (0001) surface of the crystal. The step provides the site for perpetual growth. The growth continues and the step spirals around the axis of screw dislocation. This causes the twins to grow periodically. When the first and the last layers of the growth step containing twins are in the different stacking sequence, the polytypes with hexagonal symmetry are generated. When the bottom and the top layers are in the same orientation *i.e.* *A*, *A*; *B*, *B* or *C*, *C*, the spiral growth produces polytypes with rhombohedral symmetry (Krishna & Verma, 1965). Thus the 14*H* polytype with Zhdanov symbol (77) can generate from the faulted 2*H* polytype as follows:

$$\begin{array}{r}
h\ h\ h\ h\ h\ h\ h\ k\ h\ h\ h\ h\ h\ h \\
A\ B\ A\ B\ A\ B\ A\ \underline{B}\ C\ B\ C\ B\ C\ B \\
\downarrow\qquad\qquad\qquad\qquad\qquad\qquad\qquad \\
C\ A\ C\ A\ C\ \underline{A}\ B\ A\ B\ A\ B\ A \\
\downarrow\qquad\qquad\qquad\qquad\qquad \\
B\ C\ B\ \underline{C}\ A\ C\ A\ C\ A\ C \\
\downarrow\qquad\qquad\qquad\quad \\
A\ \underline{B}\ C\ B\ C\ B\ C\ B \\
\downarrow\qquad\qquad\quad \\
A\ C\ A\ C\ A\ C \\
\downarrow\qquad\quad \\
B\ A\ B\ A \\
\downarrow\quad \\
C\ B \\
k\ k\ k\ k\ k\ k\ k\ h\ k\ k\ k\ k\ k\ k
\end{array}$$

(I) Slip at alternate layers

or

$$A\ B\ C\ A\ B\ C\ A\ \underline{B}\ A\ C\ B\ A\ C\ B,\ A\ B$$

(II) Spiral growth

or 14*H* (77).

The origin of rhombohedral polytypes can be worked out similarly.

It should be noted that the faults in the original $2H$ crystals have been assumed to be growth faults. If, on the other hand, the deformation faults are assumed to be present, the aforesaid mechanism would lead to the polytypic structures which contain '1' in the Zhdanov symbol. However, as '1' is hardly ever observed in ZnS polytypes, the contribution of the deformation faults has been neglected.

Discussion and conclusion

The results derived on the consideration of f.c.c. type microtwins along the $\langle 111 \rangle$ axes seem to be in close conformity with the structural characteristics of the ZnS polytypes observed in practice. It should be noted that in contrast to Mardix *et al.* (1968) and Daniels (1966), the cause of the polytypic growth is assumed to take place during the growth period but not at a stage when the crystals have already grown. As speculated, the type of paired numbers (n_1, n_2) in the Zhdanov symbol and percentage, p, of the layers in f.c.c. stacking sequence can completely be represented by the twin model. The value of p which is found always to be equal to or greater than 50% probably implies that the polytypic growth in ZnS results in requirement of complete transformation from the $2H$ to the $3C$ structure. However, the completion of the transformation is prevented and the process of slip (at alternate layers) accompanied by screw dislocations causes the faulted $2H$ structure to transform into periodically repeated f.c.c. type twins or polytypes. This case seems to differ from the polytypic growth in CdI_2. As shown in Table 2, p is in almost all cases equal to or less than 50% and normally contain the (11) and (22) units. Thus in this compound the polytypic growth can be treated as the consequence of structural transformation in the $4H$ and $2H$ structures by the dislocation mechanism.

Table 2. CdI_2 *polytypes*

Sample No.	Ramsdell notation	Zhdanov notation	% layer in f.c.c. orientation
1	$2H$	(11)	00·0
2	$4H$	(22)	50·0
3	$6Ha$	(2211)	33·3
4	$6Hb$	(33)	66·6
5	$8H$	$(22)\ (11)_2$	25·0
6	$10H$	$(22)_2(11)$	20·0
7	$12Ha$	(222123)	50·0
8	$12Hb$	(21211212)	33·3
9	$12Hc$	$(22)_2(11)_2$	33·3
10	$14H$	$(22)_3(11)$	42·9
11	$22Hc$	$(11)_5(2211)_2$	18·2
12	$26Hc$	$2(11)_2 2(11)_3 2(11)_2 2(11)_2$	15·4
13	$26Hd$	$(22)_6(11)$	46·1
14	$28H$	$(22)_6(11)_2$	42·8
15	$8H$	(121121)	25·0
16	$24Hg$	$(2222211)_2$	41·7
17	$12R$	$(13)_3$	50·0
18	$30R$	$(221212)_3$	40·0
19	$42R$	$(22221212)_3$	42·8

The mechanism proposed in this paper differs considerably from those proposed by Daniels (1966) and Mardix, Kalman & Steinberger (1968). In these cases, the mechanisms are assumed to operate after the time when the crystals have completed their growth. In the case of Daniels the cause of the periodic occurrence of faulting is quite clear while in the case of Mardix *et al.* (1968) the process which causes the slip to occur periodically is not mentioned. However, the periodic occurrence of faultings alone is not enough to explain the polytypic growth in a compound. The generation of various structures in terms of Zhdanov symbol which usually occur in polytypes of a given compound, should also be explained at the same time. In the case of Daniels (1966) the presence of the (11) units is inherent but it is hardly ever observed in ZnS polytypes. It is also not very difficult to see that the process of periodic slips in most of the cases will generate polytypes (starting from defect-free $2H$ crystals) which will certainly contain the (11) units or at least 1 in the Zhdanov symbol. It should be pointed out, therefore, that both of these mechanisms will generate polytypes from the $2H$ phase, but the type of structures observed in ZnS polytypes generally do not result from these mechanisms. Contrary to the above, the mechanism presented in this paper operates while crystals of the $2H$ type are growing, and the structures generated from faulted $2H$ crystals are in close conformity with the structures of observed polytypes.

In the present treatment the contribution of the deformation faults has been neglected. Normally only two kinds of stacking fault (*i.e.* extrinsic and intrinsic faults) can be associated with the h.c.p. structures. While the extrinsic fault can be formed by inserting a close-packed layer, the intrinsic faults can be introduced in h.c.p. structures in the following two ways:

(i) By only shearing the part of perfect h.c.p. structures, *i.e.*

$$\begin{array}{ccccccccccl}
 & A & B & A & B & A & B & A & B & & \\
 & A & B & A & B & \overline{C} & \overline{A} & \overline{C} & \overline{A} & & \\
 & h & h & h & k & k & h & h & h & & (h\ k\ \text{notation}) \\
(& 1 & 1 & & \overline{3} & & 1 & 1 & &) & (\text{Zhdanov notation})
\end{array}$$

(ii) By removing a close packed layer from the perfect h.c.p. structures and then by shearing, *i.e.*

$$\begin{array}{ccccccccccl}
 & & & & & \uparrow & & & & & \\
 & A & B & A & B & A & B & A & B & & \\
 & A & B & A & B & & B & A & B & & \\
 & A & B & A & B & & \overline{C} & \overline{B} & \overline{C} & & \\
 & h & h & h & k & & h & h & h & & (h\ k\ \text{notation}) \\
(& 1 & 1 & & \overline{2} & 1 & 1 & & &) & (\text{Zhdanov notation})
\end{array}$$

The intrinsic faults produced according to (i) and (ii) are known as deformation and growth faults, respectively. However, these names are misleading as the growth faults may appear during deformation and the deformation faults during growth of the crystals. From the point of view of stacking fault energy, the growth faults are energetically more economic than deformation and extrinsic faults (Hirth & Lothe, 1968). Therefore the major contribution to the growth of polytypes is expected from the growth faults. The contribution of faulting due to deformation or slip, however, may not be neglected completely at a later stage when the crystals are cooling. Probably, this is the reason why a few exceptional polytypes ($9R$, $12R$ and $21R$) are found to contain 1 in the Zhdanov symbol with p less than 50%. These polytypes may result from the periodic slips in the close-packed planes of some other polytypes and their structures may be explained according to the present mechanism. Therefore, the polytypes $21R$ may originate from another polytype $7H$ with Zhdanov symbol (52) as follows:

$$\begin{array}{ccccccccccccccccccccccccccccc}
A&B&C&A&\underline{B}&C&B&A&B&C&A&\underline{B}&C&B&A&B&C&A&\underline{B}&C&B&A&B&C&A&\underline{B}&C&B&A\\
&&&&\downarrow&&&&&&&&&&&&&&&&&&&&&&&&\\
&&&&C&A&C&B&C&A&B&\underline{C}&A&C&B&C&A&B&\underline{C}&A&C&B&C&A&B&\underline{C}&A&C&B\\
&&&&&&&&&&&\downarrow&&&&&&&&&&&&&&&&&\\
&&&&&&&&&&&A&B&A&C&A&B&C&\underline{A}&B&A&C&A&B&C&\underline{A}&B&A&C\\
&&&&&&&&&&&&&&&&&&\downarrow&&&&&&&&&&\\
&&&&&&&&&&&&&&&&&&B&C&B&A&B&C&A&\underline{B}&C&B&A\\
&&&&&&&&&&&&&&&&&&&&&&&&&\downarrow&&&\\
&&&&&&&&&&&&&&&&&&&&&&&&&C&A&C&B\\
A&B&C&A&C&A&C&B&C&A&B&A&B&A&C&A&B&C&B&C&B&A&B&C&A&C&A&C&B
\end{array}$$

or $21R$ $(3112)_3$.

(Slip has occurred at the underlined layers.)

The frequency with which a polytype is found will depend upon the frequency at which slip at alternate layers and screw dislocation take place simultaneously in the $2H$ type crystals containing growth faults. The faulting at the later stage of the growth of polytypes will tend to transform a polytype into another ordered (polytype) or disordered structure.

The problem of the stability of ZnS polytypes generated by the proposed mechanism can also be analysed in terms of Mitchell's (1957) theory of screw dislocation. According to this theory, the screw dislocations in SiC polytypes ($6H$, $4H$ and $15R$) are accompanied by a horizontal shift and a corresponding gap in the substratum. The size of the gap (or horizontal shift) depends upon the Burgers vector strength of the screw dislocation. Mitchell in his work assumed that only small gaps like R_1, R_2 and N in a $6H$ structure can lead to stable polytypes. From his assumption, therefore, it appears that the smaller gap size will lead to more stable structures. Taking this assumption as correct, one can notice that the N type of gap, which is smallest in size and produced by screw dislocations with the Burgers vector strength equal to or a multiple of the unit cell heigth of the parent structures, will lead to most stable polytypes. However, polytypes generated in this case will assume the same structures as the parent polytypes. Applying this to ZnS, it is evident that the polytypic structures produced by screw dislocations with the Burgers-vector strength equal to the unit-cell height of f.c.c. microtwins, will be more stable than those structures produced by the dislocation with a Burgers vector strength equal to a fraction of unit cell height of the proposed microtwins. In other words the growth of the f.c.c. microtwins as a whole is more probable because this involves the screw dislocations with the smallest possible gap in the substratum (f.c.c. twin).

Until this paper, no direct observation supporting the mechanism proposed above had been made. However, it should be pointed out that this mechanism will produce morphological features on the prismatic planes similar to those discussed by Daniels (1966) and Mardix, Kalman & Steinberger (1968). If the screw dislocation mechanism holds good for the growth of ZnS crystals, the observation of spirals on the (0001) face of the polytypes can be taken as evidence in favour of it. From the consideration discussed in § 3, it is highly probable that the proposed mechanism will leave some markings of the spiral growth on the (0001) face of the polytypes. In this respect, the observations of spirals by Bhide (1957) and Votava, Amelinckx & Dekeyser (1953) on ZnS crystals may be taken as indirect and partial verification of the proposed mechanism.

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A Generalized Polynomial For the Extraction of the Periodic Vector Set From the Patterson Function

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Crystal-structure analysis *via* the Patterson function may be considered as consisting of two distinct steps. In the first step, the weighted periodic vector set is determined by establishing the location of each peak in the Patterson function. In the second step, the weighted periodic vector set is analysed to determine the crystal structure. The second step apparently offers little difficulty, since existing procedures for the analysis of periodic vector sets appear to be capable of dealing with complex structures, provided of course that the vector set is accurately determined. Unfortunately, a general and powerful method for the location of peaks in the Patterson function has not yet been developed and therefore it is the first step in the solution process which now prevents the formulation of a general method of structure analysis *via* the Patterson function. Such a method would be extremely useful, since the Patterson function is not restricted to centrosymmetric structures. In the present paper a way of representing the Patterson function as a linear generalized polynomial in a system of independent interatomic functions is developed. The coefficients of this polynomial determine the weighted periodic vector set. This approach, therefore, reduces the problem of extracting the periodic vector set from the Patterson function to a relatively simple problem in linear approximation, namely the determination of the coefficients of a generalized polynomial.

Introduction

During the past fifty years many methods for the solution of crystal structures have been proposed. These existing methods are all limited to crystals with special characteristics, and a general method, capable of dealing with virtually any sort of crystal in a routine manner, remains to be discovered.

In order to formulate a general and practical method of structure analysis, one would naturally think of working in terms of the Patterson function, since this function is not restricted to centrosymmetric structures. It is now well known that a weighted periodic vector set (Buerger, 1959) can be associated with the Patterson function of an arbitrary crystal. In the following discussion, weighted vector sets will often be referred to simply as periodic vector sets, since unweighted sets will never be considered. For a crystal containing N atoms per unit cell, the periodic vector set consists of N periodic images of the crystal structure. The essence of the phase problem lies in the separation of the various points of the periodic vector set into these images. This separation can be accomplished for periodic vector sets by the image-seeking method of Buerger (1950), even though this method was originally devised in terms of non-periodic vector sets. Tokonami & Hosoya (1965) have developed a different procedure for unravelling periodic vector sets. Their method depends explicitly on certain periodic characteristics of the periodic vector sets. It also offers certain computational advantages over the image-seeking methods.

These considerations indicate that crystal-structure analysis *via* the Patterson function may be viewed as consisting of two distinct steps. In the first step, the peaks in the Patterson function are located; this determines the periodic vector set. In the second step, the periodic vector set is solved to yield the crystal structure. Unfortunately we do not have, at the present time, a general and practical method for the location of peaks in the Patterson function. Consequently, it is the first step in the solution process, that of locating the peaks in the Patterson function, which now prevents the development of a general method of structure analysis in terms of the Patterson function. It would seem that if