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Analysis of the Layer Sequence for Crystals with Stacking Faults by the Method of Structural Models: Comparison with the Direct Method of Farkas-Jahnke*

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A development of a method of analysis based on models for crystals with complex polytypic structure is presented. The method is applicable to the analysis of structures consisting of the polytypes 2*H*, 4*H* 6*H* and 10*H* and of fragments of a *DS* structure appearing in ZnS and ZnS solid solutions. A discussion of the direct method of Farkas-Jahnke for characterizing structures with stacking faults is presented and it is shown that interpretation of the real sequence by the direct method is ambiguous. The mechanism of formation of the crystals investigated is discussed from the point of view of the results obtained.

Introduction

In the previous paper (Pałosz & Przedmojski, 1976*a*) the possibility of applying methods of analysis to crystals with stacking faults (Wilson, 1942; Jagodzinski, 1949; Kakinoki & Komura, 1965; Kakinoki, 1967) was discussed. Differences between theoretical and experimental curves of intensity distribution were found. To explain the appearance of maxima on experimental curves which are not reflexions connected with polytypes a newly defined *DS* structure was proposed (Pałosz & Przedmojski, 1976*b*). On the basis of this *DS* structure a composition of complex structures with stacking faults from simple polytype cells (2*H*, 4*H*, 6*H* and 10*H*) and of *DS* fragments was proposed. The purpose of this paper is a complete presentation of the method of structural models applied to the analysis of structures with stacking faults appearing in ZnS and ZnS solid solutions.

From structural models of complex structures, calculations of theoretical curves of intensity distribution were performed. With their help a few hundred ZnS and ZnS solid-solution crystals were analysed. It was found that: (1) theoretical intensity curves are applicable to structural analysis; (2) on the basis of the proposed description of structures with stacking faults, reproducible and unique determinations of the stacking sequence of crystals are obtained.

A comparison of the direct method for characterizing structures with stacking faults (Farkas-Jahnke, 1973*a*, *b*) with the proposed method of structural models will be discussed. It will be shown that while the results obtained in the Farkas-Jahnke method do not give a unique stacking sequence in the crystals, the proposed description using a *DS* structure yields the correct answer. A short description of our experimental results will be presented and the possibility of their interpretation based on existing theories of polytype crystal growth mechanisms will be discussed. In these discussions the possibility of appearance of a mechanism of incidental formation of polytype cells will be pointed out.

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A short description of the Farkas-Jahnke direct method

The procedure of structure determination by the direct method is given by Dornberger-Schiff & Farkas-Jahnke (1970), Farkas-Jahnke & Dornberger-Schiff (1970), Dornberger-Schiff, Schmittler & Farkas-Jahnke (1971), and Farkas-Jahnke (1973*a*,*b*). In this method polytypic structures are regarded as built up of structure elements consisting of $(p+1)$ layers. The $(p+1)$ layer sequence is denoted in a binary system as a set of p digits: the digit 0 corresponds to $-$ and the digit 1 to $+$ in Hägg's notation. For periodic structures (polytypes), structural analysis is based on determining the rates of occurrence $[\gamma]_p$ of binary sequences of length p (γ_p) in the structure, from which it is then possible to reproduce the full layer sequence of the polytype. A mathematical analysis is carried out on the basis of intensity measurements of a characteristic row of reflexions, *e.g.* 10.*L*. In structures with stacking faults, *i.e.* the lack of any periodicity along **c**, the broadened curve obtained by photometering of 10.*L* row of reflexions is treated as the result of the overlapping of reflexions of a hypothetical N-layer lattice. The intensities obtained from the curve for consecutive values of L/N (for L from 0 to N) are accepted as the intensities of reflexions from a structure with N layers in a period. The determination of the structure consists of finding its set of $[\gamma]'_p$ values where $[\gamma]'_p=[\gamma]_p/N$.

Construction of structural models

The intensity curves which form the foundation for structural analysis were obtained from structural models built up from 200 ± 5 layers. These models con-

sist of simple polytype cells and of *DS* fragments, where the *DS* structure was defined as the sequence of Zhdanov symbols $\ldots n_1 n_2 n_3 \ldots$ showing no periodicity. The structure of each model is described by three independent parameters: (i) The percentage of layers arranged in simple polytype cells (25%2*H*, 45%10*H*, *etc.*). (ii) %*h DS*, *i.e.* the percentage of hexagonal layers appearing in fragments of the *DS* structure. (iii) The size of monopolytype fragments, *i.e.* the average number of polytype cells occurring one after another in the structure.

From the above it is possible to find two additional parameters: (iv) The percentage of *DS* structure in the whole model. (v) %*h* (hexagonality), the percentage of hexagonal layers in the whole model.

The additional quantity which can be calculated from photometric curves is (vi) the parameter determining the ratio of the number of layers in the positive (N_+) and negative (N_-) sequences.

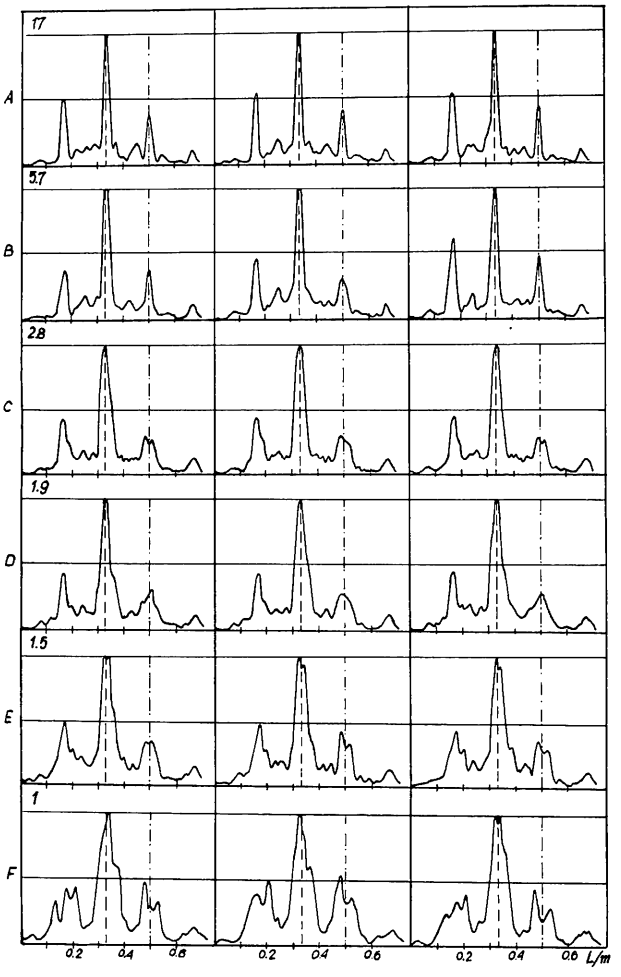


Fig. 1. Diagram of theoretical curves of intensity distribution along a row of 10.*L* reflexions for the structure 6*H*(50% layers)+*DS*(35%*h*) obtained for models with 6*H* fragment sizes from 17 cells to 1 cell.

With the help of the above parameters it is possible to reproduce an equivalent structure.

The real layer sequence of crystals can be presented in the form of fragments of a *DS* structure (with a defined %*h DS*) occurring next to fragments composed of simple polytype cells. For example, fragments of a *DS* structure in Zhdanov's notation can be represented as:

DS 20%*h* ...4543656454657647546537654...
DS 30%*h* ...4325424353432354324534243...
DS 50%*h* ...2131214121312412313213132...

Polytype cells are denoted: 2*H*, (11); 4*H*, (22); 6*H*, (33) and 10*H*, (55).

An example of a complex structure model of the 4*H*+*DS* type is

$$\ldots 2\,4\,(2\,2)_2\,1\,2\,3\,2\,(2\,2)_3\,3\,4\,3\,1\,2\,2\,2\,3\,2\,1\,4\,(2\,2)_3\,1\,2\,3\,(2\,2)_4\,4\,1\,2\,(2\,2)_2\ldots$$

The above model consisting of 110 layers is described by the following parameters:

(i) 55%4*H* [(15 cells × 4 layers)/110] × 100%;

(ii) *DS* 42%*h* [(21 different blocks in a + and − sequence)/(50 layers in the *DS* structure)] × 100%;

(iii) 2·5 4*H* cell {[(2+3+1+3+4+2) cells]/6 fragments} = 2·5;

(iv) 45%*DS* (100% − 55%4*H*) = 45% of layers in the *DS* structure;

(v) 46%*h* {[(21 *h* layers in *DS*) + (30 *h* layers in 4*H*)]/110} × 100%.

The description given above with three independent parameters ensures reproduction of the real stacking sequence in the structure.

Equivalent structural models for the same set of parameters

Intensity curves obtained for models of the 6*H*(50% of the layers)+*DS*(33·3%*h*) structure are shown in Fig. 1. Curves for models with identical 6*H* cell fragments lie in horizontal rows. The models differ in the arrangement of the fragments of *DS* and of 6*H* cells in the structure. For example, we consider three equivalent models: (1) $\ldots 3\,3\,1\,2\,(3\,3)_5\,3\,4\,2\,1\,3\,3_2\,5\,3\ldots$, (2) $\ldots 3\,4\,(3\,3)_3\,1\,2\,1\,3\,2\,(3\,3)_4\,5\,3\,3\ldots$, (3) $\ldots 4\,5\,1\,(3\,3)_2\,3\,1\,2\,(3\,3)_4\,2\,3\,(3\,3)_2\ldots$ Fig. 1 presents theoretical curves obtained for structures with monopolytype fragments of different sizes ranging from 17 cells occurring in one fragment of the structure to single 6*H* cells mixed into the *DS* structure.

From Fig. 1 it is possible to determine the degree of reproducibility of theoretical intensity curves for various equivalent models. Curves obtained for different models with the same parameters are not identical, but the basic shapes are preserved: (1) the positions of the main maxima (broadened reflexions of polytype 6*H*) and specific maxima (resulting from the *DS* structure), (2) width of the broadened maxima,

(3) the characteristic minima. The ratios of intensity maxima are usually constant, but deviations do occur (*e.g.* curve *B*). The diagrams presented in Fig. 1 demonstrate the high sensitivity of the method to slight differences in the stacking sequence. The dependence of the shape of the curve on the size of the monopolytype fragments allows for precise structural determination. It may be deduced from Fig. 1 that the interference pattern obtained for complex structures is not the result of a simple addition of the interference patterns of the elements of the model (here $6H$ and DS of $35\%h$). The simultaneous appearance of characteristic DS maxima and polytype reflexions can be observed in the presence of large monopolytype fragments (curve *A* and *B*); however the occurrence of single-polytype cells in the structure leads to a characteristic arrangement of maxima belonging neither to $6H$ nor to DS.

Thus, on the basis of an experimental intensity curve it is possible to estimate the sizes of monopolytype fragments in crystals, but the details of the stacking sequence can be determined only through a direct comparison of that experimental curve with a set of theoretical curves.

Structure of the crystals investigated

It was found that the following types of structures occurred in the crystals investigated: $2H+4H$, $2H+6H$, $4H+6H$, $2H+4H+6H$, $2H+DS$, $4H+DS$, $6H+DS$, $10H+DS$, $2H+4H+DS$, $4H+6H-DS$, $2H+4H+6H+DS$, $6H+10H+DS$ and DS.

The types of the analysed structural models were determined on the basis of the results of initial structural analysis. The appearance of broadened polytype reflexions on the experimental intensity curves suggested the presence of only $2H$, $3C$, $4H$, $6H$ and $10H$ polytypes. Since the accuracy of determination of the number of layers in the polytype structures can be estimated to be about 5% it is not possible to exclude the presence of other simple polytypes up to a content of about 10%, especially when present in very small fragments. Cells of several polytypes often occurred in one crystal simultaneously, forming one of the above mentioned types of structure.

The theoretical curves obtained for different types of structures are arranged in diagrams. Fig. 2(*a*) represents a fragment of the diagram of theoretical curves obtained for the $(2H+DS)$ type structure. The number in the top left-hand corner of each curve describes the average number of $2H$ cells occurring one after another in the model. Fig. 2(*b*) and (*c*) presents the theoretical curves for structures with different average $2H$ fragment size (for the same $\%2H$ in the model). Fig. 3 presents photometric curves obtained for three different crystals, whose structural determination was accomplished from the theoretical curves in Fig. 2.

The structures of crystals (*a*), (*b*) and (*c*) are com-

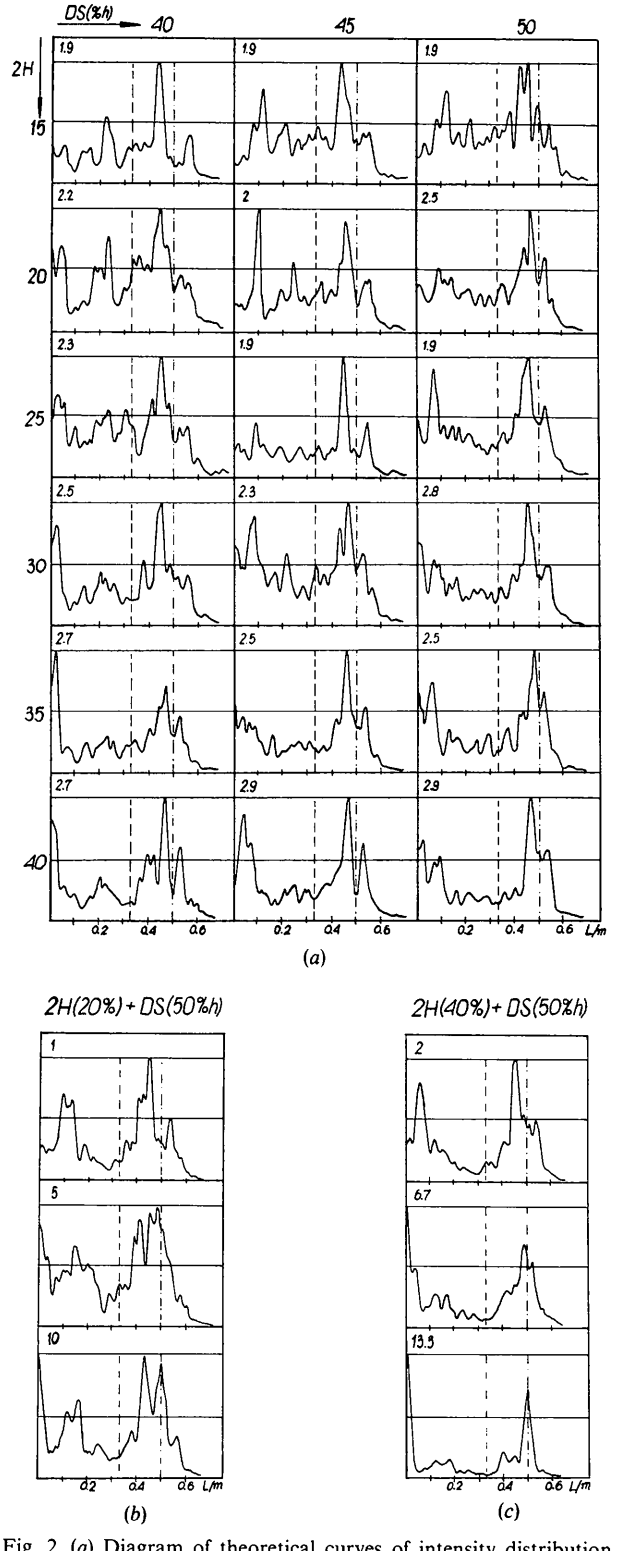


Fig. 2. (*a*) Diagram of theoretical curves of intensity distribution along a row of 10.*L* reflexions obtained for the structure type $2H$(15–40% of layers)$+DS$(40–50%h). (*b*) Theoretical curves of the structure $2H$(20% of layers)$+DS$(50%h) with fragments 1, 5 and 10 $2H$ cells. (*c*) Theoretical curves of the structure $2H$(40% of layers)$+DS$(50%h) with fragments of 2, 6·7 and 13·3 $2H$ cells.

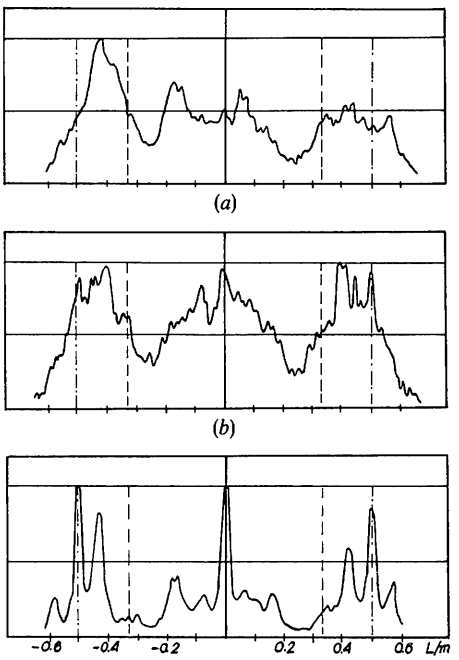


Fig. 3. Photometric curves of a row of 10.L reflexions for crystals with $2H+DS$ structure.

parable, apart from large differences in intensity distributions. The above structures differ in the sizes of $2H$ fragments. We shall describe the experimental curves in Fig. 3.

Curve (a)

Distinct maxima for L/m of about 0·05, 0·15–0·20, 0·40–0·45 and 0·50–0·55 characteristic for a $2H+DS$ (50%h) structure are observed. In spite of the lack of reflexions $2H(L/m$ 0·00 and 0·50) this structure can be described as $2H$ (about 20% of layers)$+DS$(40–50%h) with fragments of about two $2H$ cells.

Curve (b)

Broadened DS maxima are observed on the curve in positions similar to curve (*a*), but there are also $2H$ reflexions, so that one can expect larger fragments of $2H$ cells. This structure may be described as $2H$(20–25% of layers)$+DS$(about 50%h) with fragments of about five $2H$ cells.

Curve (c)

It is possible to discern characteristic DS maxima and narrow $2H$ reflexions on the curve. By comparison of curve 3(*c*) with curves 2(*b*) and 2(*c*) this structure can be described as $2H$ (about 30% of layers)$+DS$ (50%h) with fragments of about 10–15 $2H$ cells.

Among the theoretical curves presented in Fig. 2 none can be considered identical with the experimental curves shown in Fig. 3. The structural models include only part of the possible layer sequences. For this reason a given experimental curve does not always correspond to a single theoretical curve. The set of theoretical curves enables one to give limits within which the real stacking sequence of a crystal may be placed.

On the basis of theoretical curves for the $6H+DS$ structure (Fig. 1) it is possible to determine the structure of crystals for which photometric curves were shown in Fig. 5(*b*) in the previous paper (Pałosz & Przedmojski, 1976*b*). The structures of both crystals can be described as $6H$(50%)$+DS$(35%h); however the structure with fragments of about 1·5 cells corresponds to the first curve, whereas the structure with 2-cell fragments corresponds to the second. Both curves agree well with the theoretical curves.

The theoretical curves for the above mentioned structure types allowed us to carry out a full analysis of the structures occurring in ZnS and ZnS solid solutions. A discussion of the structure of crystals in relation to their chemical composition for ZnS.CdS and ZnS.ZnSe crystals was presented by Kozielski (1975)

Table 1. *Values of* $[\gamma]_4$ *for two models*

Model I of 202 layer structure

$4H$ (3·96%)$+6H$ (5·94%)$+DS$ (43·96%h), $\alpha=0{\cdot}5$

Stacking sequence

1 3 2 3 1 4 1 2 3 3 2 3 1 2 2 3 1 3 2 3 2 3 1 4 2 3 2 3 1 2
1 3 2 3 1 3 2 3 2 3 2 3 1 3 1 3 1 3 2 3 1 3 1 3 2 3 3 1 4 1
3 2 3 3 2 3 1 2 2 3 1 3 2 3 2 3 1 3 2 3 2 3 1 3 1 3 2 4

Model II of 192 layer structure

$6H$ (25%)$+DS$ (29·17%h), $\alpha\neq0{\cdot}5$

Stacking sequence

2 6 2 5 3 3 3 4 3 5 2 3 3 3 2 4 3 2 4 3 2 3 3 5 3 5 2 6 3 3
4 3 2 3 3 3 2 4 3 4 3 5 $(3\,3)_2$ 2 6 2 3 5 3 3 4 3 2 3

Sequence	$[\gamma]_4$ calculated from the model	$[\gamma]_4$ obtained by Farkas-Jahnke
Model I		
0000	3	2·88
0001	38	37·49
0010	19	18·77
0011	23	21·23
0100	19	18·77
0101	–	1·68
0110	20	16·92
0111	5	6·54
1000	38	37·49
1001	4	2·51
1010	–	1·68
1011	2	2·22
1100	23	21·23
1101	2	2·22
1110	5	6·54
1111	1	3·83
Model II		
0000 1111	15	16·3
0001 1110	23	22·58
0010 1101	–	0·13
0011 1100	29	28·5
0100 1011	–	0·13
0101 1010	–	0·13
0110 1001	6	5·85
0111 1000	23	22·58

(the concept of a *DS* structure was not used in that paper).

A comparison of the Farkas-Jahnke direct method for characterizing structures with stacking faults with the method of structural models

The theoretical curves obtained on the basis of structural models were tested by Farkas-Jahnke (1975). The comparison of the methods consists of finding the values $[\gamma]_{2,3,4}$ by the direct method based on the analysis of the intensity curve obtained for the structural model, and comparing them with the values found directly from the known stacking of the layers of the model. Such a comparison was made for several models. In Table 1 the values of $[\gamma]_4$ calculated for two models are shown.

DS		
DS		
DS	occurring in the structure type	
DS		$6H+10H+DS$

The parameters found by the Farkas-Jahnke method agree well with those obtained from the model which indicates the correct calculation of $[\gamma]_4$ values in the direct method. However, the determination of the layer sequence in the structure by use of $[\gamma]_4$ is not unique. For example the layer sequences of the structure obtained from the set of $[\gamma]_4$ values for model II are

(1) 64232733633242423432432334335 4
(2) 7524524523343234333 4(33)$_2$362
(3) 92(33)$_6$28337332263322
(4) 722(44)$_4$22(33)$_2$552(33)$_2$2335
(5) 52(22)$_2$(55)$_3$(33)$_5$233553 .

Applying the parameters describing the structural models built on the basis of *DS* for the above structures we obtain the values in Table 2.

Table 2. *The values of parameters of models* 1–5

The sizes of the monopolytype fragments are given in parentheses.

Structure	%2*H*	%4*H*	%6*H*	%8*H*	%10*H*	%*DS*	%*h DS*	%*h*
1	–	–	25 (1)	–	–	75	27·8	29·2
2	–	–	25 (1·33)	–	–	75	27·8	29·2
3	–	8·3 (1)	57·2 (3·5)	–	–	35·4	17·6	29·2
4	–	8·3 (1)	21·2 (2)	33·3 (4)	10·4 (1)	16·7	25	29·2
5	–	8·3 (2)	37·5 (3)	–	41·6 (2)	12·5	33·3	29·2
Initial model	–	–	25 (1·14)	–	–	75	29·2	30·2

This comparison shows that there are many possibile interpretations of the stacking sequence in a crystal which can be obtained from the calculated numbers of structure elements consisting of five layers in the structure.

Mechanism of structure formation

The analysis of the structure of ZnS and ZnS solid solutions suggests a mechanism of structure formation. ZnS and ZnS solid solutions obtained by the Bridgman method (Kozielski, 1975) and ZnS crystals obtained by chemical transport (Pałosz, 1975) were analysed. In both cases the existence of structures of a similar type was determined. It is characteristic that the appearance of different simple polytype cells was usually connected with the occurrence of *DS* with a hexagonality close to the percentage of *h* layers in the polytype cells as follows:

$2H+DS$		50%	
$4H+DS$	had about	35%	*h* layers .
$6H+DS$		30%	
$6H+10H+DS$		20%	

It seems that the formation of cells of particular simple polytypes proceeds to a large degree in an incidental manner as the result of the two 1, 2, 3 or 5-layer blocks of the same size appearing one after another. For instance, since the largest percentage of 3-layer blocks occurs in structures with hexagonality of about 30%*h* (the average size of the layer blocks is about 3) a maximum of the occurrence of 6*H* cells in the structure should be observed in this range. This conclusion is in agreement with observations. Similar agreement is found for the occurrence of 10*H* cells (*DS* about 20%*h*) as well as 4*H* cells (*DS* about 35–40%*h*). In structures with a hexagonality above 50%*h* the increase of the number of 1-layer blocks is connected with the occurrence of 2*H* cells. The observed sizes of monopolytype fragments, usually from 1 to 3 cells, also point to the incidental character of formation of polytype cells.

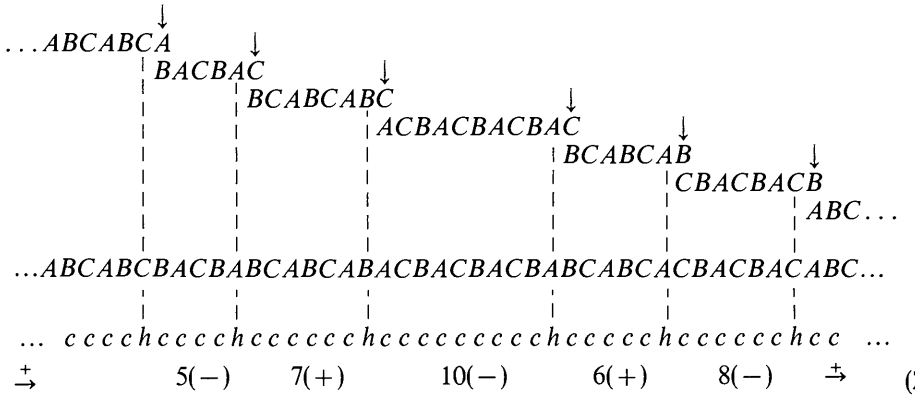
The observed relation between the hexagonality of the structure and the hexagonality of polytypes which appear explains why structures in which 2*H* and 10*H* cells as well as 10*H* cells with *DS* 50%*h etc.* (that is structures with various degrees of hexagonality) do not occur simultaneously.

The mechanism of polytype formation in ZnS crystals has been the subject of many papers (Verma & Krishna, 1966; Daniels, 1966; Mardix, Kalman & Steinberger, 1968; Alexander, Kalman, Mardix & Steinberger, 1970; Rai, 1971, 1972) in which the formation of multilayer polytypes in the process of crystal growth from the vapour phase was mainly discussed. The ZnS crystals usually investigated were synthesized from the vapour phase at about 1200 °C, *i.e.* above the temperature of the $3C \rightarrow 2H$ phase transformation (about 1025 °C). At this temperature the 2*H* phase is supposed to be more stable. The mentioned theo-

ries are based on the assumption that at the temperature of crystallization the stable phase is the 2*H* structure, which, as a result of transformation, gives more complex polytype structures, in particular multilayer polytypes. The important part of some theories is the assumption of the occurrence of an axial screw dislocation (Frank, 1951; Mitchell, 1957) causing the repetition of structure fragments and the formation of multilayer polytypes. The fact that in the crystals investigated we observed the domination neither of 2*H* structure nor of multilayer polytypes both in the pure ZnS crystals (Pałosz & Przedmojski, 1975) and in ZnS solid solutions suggests a different mechanism of crystal growth than that which occurs in crystallization from the vapour phase.

It may be that, with the Bridgman method, the formation of a 3*C* structure is more probable. At the same time, the final crystal structure may form during the growth or during cooling from the growth temperature to room temperature. Ebina & Takahashi (1967) investigated ZnS crystals obtained by the Bridgman method for different cooling rates of 67, 10, and 5 °C min^{-1}. They found that the cooling rate does not influence the crystal structure. Therefore it is possible that the final structure of the crystals is formed during their growth. As the final structure is the cubic phase, the conditions of growth have to favour the formation of the 3*C* structure.

The analysis of the structure of pure ZnS crystals (Pałosz & Przedmojski, 1975) showed that the growth of a 3*C* structure is disturbed on average at every 15 layers, *i.e.* every 15th layer is a hexagonal layer (about 7% hexagonal layers in the structure). In pure ZnS the occurrence of hexagonal layers may be influenced by growth conditions such as temperature inhomogeneity, mechanical stresses (pressure about 100 atm), presence of trace impurities *etc.* In solid solution the occurrence of hexagonal layers is connected with the presence of foreign atoms in the ZnS lattice. The appearance of a hexagonal layer causes the change of the growing sequence $+(-)$ to $-(+)$ leading to the formation of a structure according to the model $\ldots(m_1 \,.\, c)h(m_2 \,.\, c)h(m_3 \,.\, c)h\ldots$ *etc.* corresponding to the proposed *DS* structure. Such a mechanism may be presented as follows:



(Zhdanov notation).

Appearance of non-periodical stresses during the growth (marked by arrows in the proposed model of growth) on the surface of the crystal causes the growth of the *DS* structure. As a result of the appearance of identical 1, 2, 3 and 5-layer blocks one after another the 2*H*, 4*H*, 6*H* and 10*H* cells are formed.

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