maps computed with equation (3). The NRC Crystallographic programs (Ahmed, Hall, Pippy & Huber, 1966) and *ORFLS* were used in the computations. The data were collected on a Picker FACS-1 System with molybdenum radiation (graphite monochromator). This work was supported in part by grant MA-3406 to M.N.G.J. from the Medical Research Council of Canada and in part by the National Research Council of Canada grant (A-172) to R.U. Lemieux for support to L.T.J.D.

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A New Direct Method for Characterizing Structures with Stacking Faults, Built up from Translationally Equivalent Layers. I. Faults in Stackings of Three and Four Layers

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The direct method for determination of the stacking sequences of periodic polytypes has been successfully applied to the calculation of structural characteristics of stacking-faulted lattices built up of translationally equivalent layers. From the intensity distribution along row-lines of indices $h-k \neq 3n$ on oscillational X-ray patterns $\pi'(m,p)$ sets were calculated, which give the relative rate of occurrence of the related stacking vectors. Formulae are derived for calculating cyclicity, hexagonality and the relative rate of occurrence of four-layer stackings using the $\pi'(m,p)$ values. It is shown that this method may be used also to determine directly the α and β fault parameters used by Jagodzinski.

Introduction

Because of the practical importance of materials with structures built up of translationally equivalent layers, several theories and methods have been worked out since the early days of X-ray diffraction methods to make possible the characterization of their faulted structures (Warren, 1941; Hendricks & Teller, 1942; Gevers, 1952, 1954; Kakinoki & Komura, 1952; Paterson, 1952; Johnson, 1963; Allegra, 1964; Sato, 1966, 1969; Kakinoki, 1967; Lele, Anantharaman & Johnson, 1967; Holloway, 1969; Lele, 1969; Lele, Prasad & Anantharaman, 1969; Lele & Rama Rao, 1970; Prasad & Lele, 1971). These methods, however, are all indirect, assuming random distribution of stacking faults. Moreover, most theories suppose the presence of only one type of stacking fault in the lattice. One method without the latter restriction is that of Jagodzinski (1949*a*, *b*, *c*). Assuming a random stacking-fault distribution and an interaction range of three interlayer spacings ('Reichweite = 3'), he determined the effect of this type of disorder on the intensity distribution of scattered X-rays. His method was partly based on earlier work of Landau (1937) and Wilson (1942). Jagodzinski's two-parameter model was further developed and applied to some practical cases, mostly for the characterization of faulted ZnS structures by Müller (1952) and Singer & Gashurow (1963), who achieved, however, a reasonably good fit between calculated and photometrically measured intensity curves for random stacking fault distribution only. Even in these cases the use of the method was rather tiresome since, being an indirect method the calculation of a set of master curves was needed to find the best fitting curve whose parameters may be characteristic of the structure.

We encountered the problem of characterizing lattices with stacking faults when investigating the structure of a great number of ZnS crystals. These crystals have been widely investigated because of their interesting polymorphic modifications. But, as has been shown by many authors (Müller, 1952; Brafman, Shachar & Steinberger, 1965; Verma & Krishna, 1966), these crystals (the natural ones and also those grown by different methods) only seldom have a completely regular structure. Besides the high-temperature hexagonal, the low-temperature cubic, and the numerous polytype modifications, the structure of the majority of the crystals contains many stacking faults. In such regions the Zn–S double layers of hexagonal symmetry are stacked perpendicularly to the hexagonal *c* axis (*i.e.* the cubic [111] direction) in such a manner that neighbouring

layers are always related to each other by a translation of $\pm\frac{1}{3}$ of the lattice distance along the orthohexagonal b axis (*i.e.* the $[1\bar{1}0]$ axis of the hexagonal lattice), but in most cases their stacking has no regularity or periodicity. The same is valid for SiC and for many other crystals built up of translationally equivalent layers.

The experimental observation that in many cases it is not possible to obtain a good fit between intensity distributions measured on X-ray patterns and those calculated by indirect methods, corresponds to our X-ray and electron diffraction investigations carried out on a great number of ZnS crystals. They proved that in many cases these structures do not contain faulted hexagonal or cubic regions, but rather a number of differently faulted polytype regions, frequently having very small dimensions parallel to the c axis, but occupying the whole diameter of the crystal perpendicular to it (Fig. 1). Even when the intensity distribution of patterns which seemed to be of a stacking-faulted cubic or hexagonal crystal were measured, the curves obtained along the row line h,k,l with $h-k\neq 3n$ showed few periodic peaks apart fom the hexagonal or cubic reflexions (Fig. 2). These periodic maxima correspond to a faulted polytype lattice. From another point of view, however, this lattice can be regarded as a structure whose faults are no longer randomly distributed; a fault migration occurs which is almost periodic.

These experimental observations, and the lack of a relatively simple method which could characterize all kinds of faulted structures, not only those with random stacking faults, led to the idea of applying the direct method for this purpose, which was originally elaborated for the structure determination of ZnS-like polytypes.

Changes in the definition of quantities used in the direct method for stacking-faulted lattices

The basic features of the above-mentioned polytype stacking sequence determining method, given in detail by Farkas-Jahnke (1966), Dornberger-Schiff & Farkas-Jahnke (1970), Farkas-Jahnke & Dornberger-Schiff, (1970), are the following:

(1) It uses a new notation for polytypes: a binary of N digits. N is the number of Zn–S double layers in one period. These layers could be translated into each other by either of the two translational vectors, $\mathbf{a}_1\,(-\frac{1}{3},\frac{1}{3},1/N)$ or $\mathbf{a}_0\,(\frac{1}{3},-\frac{1}{3},1/N)$. The row of the indices of the translational vectors constitutes a binary of N digits, which is periodic in the case of periodic polytypes (*e.g.* the notation of the $6H$ polytype in this system is 111000 ...).

(2) It employs the so-called 'stacking vectors', *i.e.* vectors with coordinates (m,p) connecting identical points in double layers p steps apart, related to each other by the translation $m/3$ along the orthohexagonal b axis (possible values $m=0,\pm 1$).

(3) It introduces a new function, the $\pi(m,p)$ Patterson-like function. The values of this function, differing from zero only at points of integer (m,p) coordinates; give the number of stacking vectors of coordinates (m,p).

(4) When using our method, the periodic structure is regarded as being built up of structure elements consisting of $p+1$ layers. It is obvious that the notation of these structure elements in the '10' system is a binary of p digits. ($p+1$ layers are connected by p translational vectors.) There exists a close connexion between the position of identical points in the first and last layer, respectively, in the structure element and the coordinates of the related stacking vector. The whole translation of the lattice during p steps in the direction **b** is congruent with the m coordinate of the stacking vector (m,p), *i.e.* the translation $=m$ (mod 3) (in $|b|/3$ units) (Fig. 3).

(5) The procedure for structure determination of periodic polytypes is the determination of the rate of occurrence of longer and longer structure elements recursively. It is clear that even the rates of occurrence of 'short' sequences (*i.e.* sequences consisting of a few layers only) are very characteristic of the structure. (The structure elements of length p will be denoted by γ_p, and their rate of occurrence by $[\gamma]_p$.)

This recursive nature of the procedure also enables us to make use of it in cases when, in the absence of real periodicity, a full determination of the structure is not possible.

These ideas could be easily applied to structures with stacking faults (Farkas-Jahnke, 1968). The binary notation of a one-dimensionally disordered structure will obviously be an almost infinite row of 1's and 0's. The stacking vectors also have their original meaning in this case. The first difficulty arises for the $\pi(m,p)$ functions; while lacking real periodicity they cannot have any meaning for the stacking-faulted lattice. It is possible, however, to overcome this difficulty by introducing a 'relative' Pattersonian function,

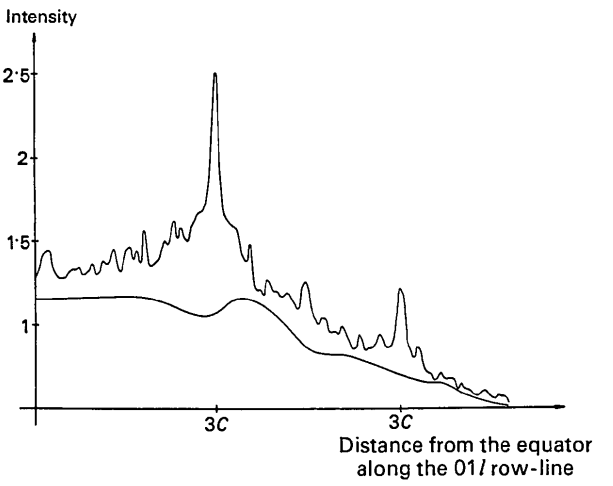

Fig. 2. Blackening distribution measured along the $01l$ row-line of the X-ray pattern of a crystal with faulted structure.

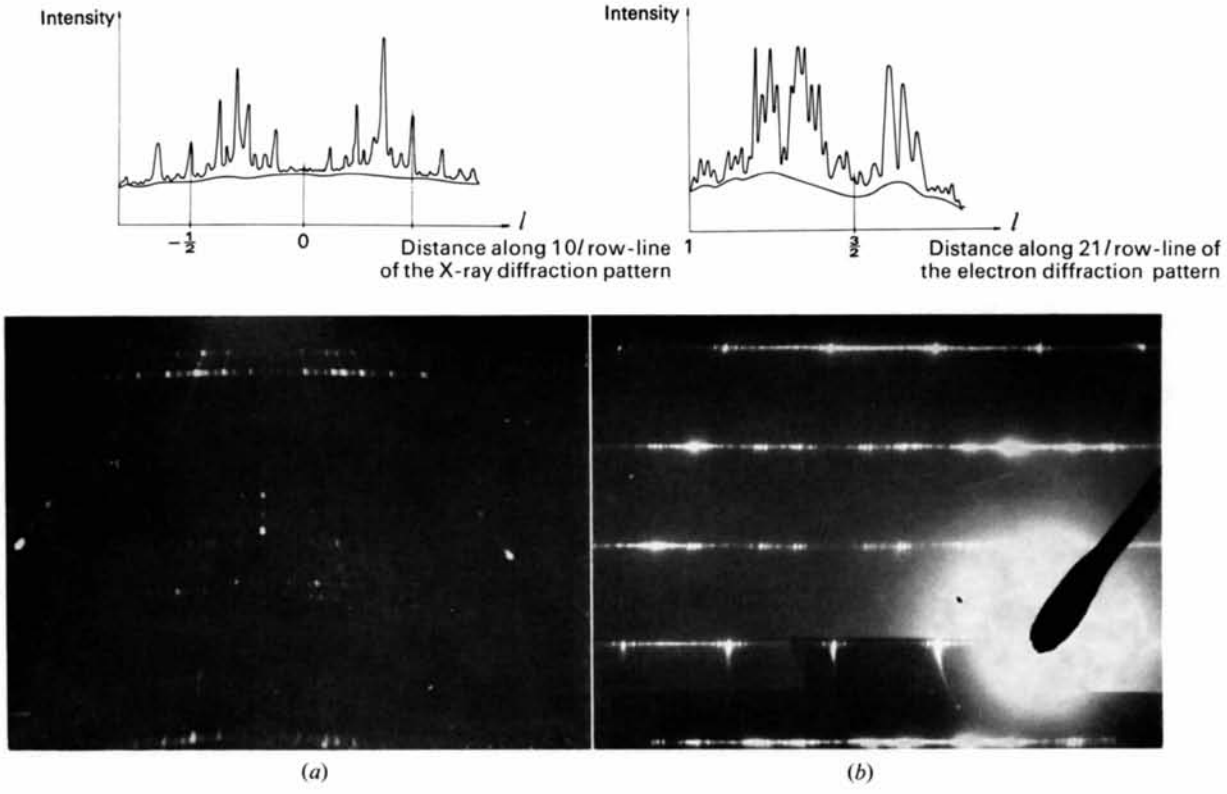

Fig. 1. (*a*) Oscillation X-ray diffraction pattern of a stacking-faulted ZnS crystal. Oscillation axis parallel to the *c* axis. Cu $K\alpha$ radiation. (*b*) Reflexion electron diffraction pattern of a ZnS crystal containing stacking-faulted polytype regions. 80 kV electrons, *c* axis of the crystal perpendicular to the electron beam.

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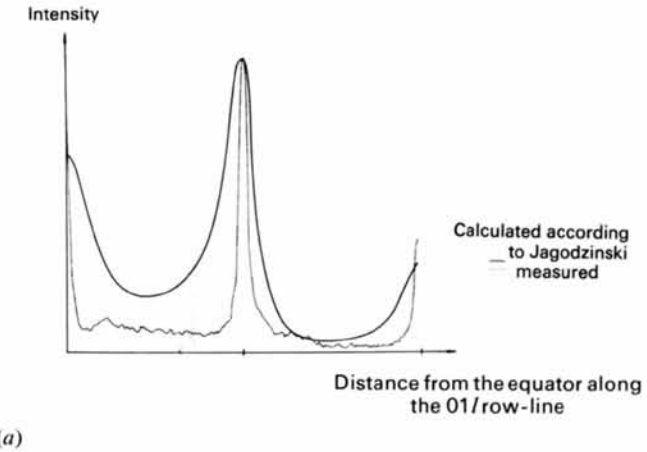
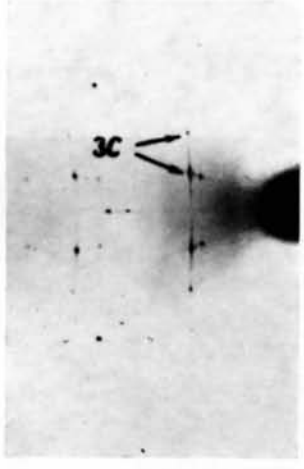
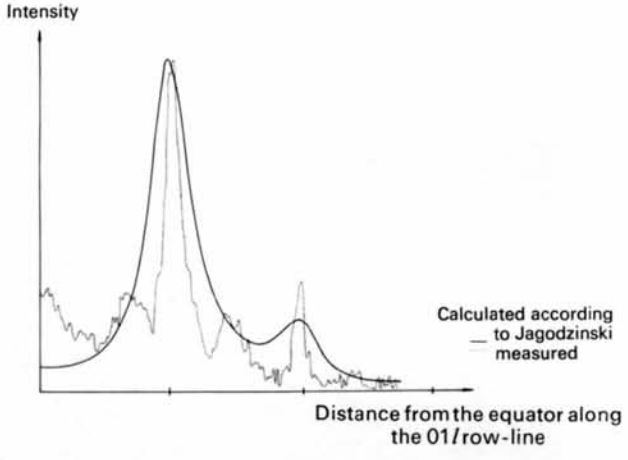
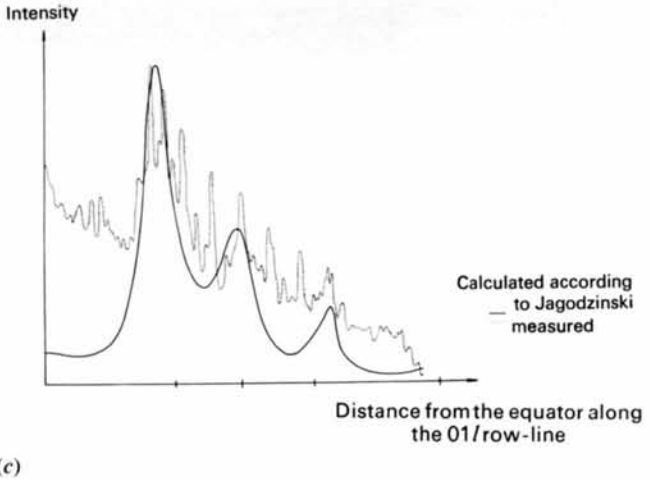


(*a*)





(*b*)



(*c*)

Fig. 6. Measured intensity distributions, X-ray patterns and calculated best fitting Jagodzinski-type curves for (*a*) a faulted hexagonal crystal, (*b*) a faulted cubic crystal, (*c*) a faulted polytype crystal.

$$\pi'(m,p)=\pi(m,p)/N \qquad (1)$$

which is now the relative number of occurrences of the stacking vector (m,p), not only within one period, but in the whole region in question. (N is the number of layers per period in a polytype and the number of layers in the investigated region of a faulted crystal.)

The faulted lattices as well as the lattice of periodic polytype are built up of structure elements of length p (denoted by γ_p) except that their occurrence lacks any periodicity this time. Therefore we have to modify our former definition of the rate of occurrence of such structure elements, $[\gamma]_p$, in a way similar to that used for the $\pi(m,p)$ functions. Only the relative rate of occurrence,

$$[\gamma]'_p=[\gamma]_p/N \qquad (2)$$

which is equal to the relative number of stacking γ_p in the whole region in question, can be used for faulted structures.

Calculation of $\pi(m,p)$ from the intensity distribution of a pattern made from a crystal with stacking faults

After introducing these new definitions for $\pi'(m,p)$ and $[\gamma]'_p$ a more serious problem arose: the calculation of $\pi(m,p)$, *i.e.* $\pi'(m,p)$ values for a stacking-faulted structure. In a periodic polytype it is defined by the equation

$$\pi(m,p)=\frac{N}{3}\left[1+2\sum_{l=0}^{N-1}\frac{|S(0,1,l)|^2}{N^2}\cos 2\pi(m/3+lp/N)\right] \qquad (3)$$

where $|S(0,1,l)|^2$ can be determined from the structure factors of reflexions along the row-line $(0,1,l)$ using the relation

$$|S(h,k,l)|^2=\frac{|F(h,k,l)|^2}{|F_o(h,k,l)|^2} \qquad (4)$$

where $F_o(h,k,l)$ denotes the known structure factor of one double layer.

In the case of stacking-faulted crystals, reflexions along row-lines for which $(h-k)\neq 3n$ are no longer separated, but are connected by a diffuse line of varying intensity. So, it is not clear what should be substituted for $|S(0,1,l)|^2$ in equation (3).

To overcome this difficulty we arrived at the following idea: choosing a value for N, we measured the blackening of the diffuse line at those points where a polytype of period length N would have given reflexions. Using equations (3) and (4), we obtain a set of $\pi(m,p)$ values. If using different N values the $\pi'(m,p)$ sets obtained do not differ very much, the set of mean values of these $\pi'(m,p)$'s can be accepted as characteristic of the stacking-faulted structure in question. In most cases the choice of N is obvious because of the periodicity of the small peaks on the diffuse lines. An example for such sets calculated from the blackening distribution shown in Fig. 2, choosing $N=24$ and 54 is given in Table 1.

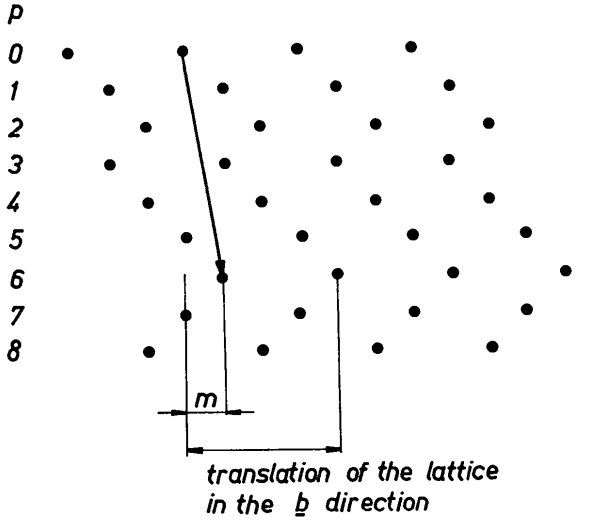


Fig. 3. Relation between the coordinates of the stacking vector (m,p) and the whole translation of the lattice during p steps.

Cyclicity, hexagonality and four-layer stackings in non-periodic structures

Already from the set of $\pi'(m,p)$'s useful information can be derived about the properties of a stacking-faulted structure. According to their definition $\pi(1,1)$ and $\pi(-1,1)$ give the whole number of 1's and 0's, *i.e.* the number of translations a_1 and a_0 in a periodic polytype. $\pi'(1,1)$ and $\pi'(-1,1)$ supply us with the corresponding relative values for the investigated region in a faulted crystal.

The difference $\pi(1,1)$–$\pi(-1,1)$ is equal to the so-called 'cyclicity' of a periodic polytype, *i.e.* the translation of the lattice parallel to the direction of the

Table 1. $\pi'(m,p)$ *values calculated from the same intensity distribution*

		$N=24$			$N=54$		
p	m	-1	0	$+1$	-1	0	$+1$
1		0·501	−0·002	0·501	0·488	0·238	0·488
2		0·350	0·301	0·350	0·377	0·247	0·377
3		0·256	0·490	0·256	0·244	0·512	0·244
4		0·366	0·268	0·366	0·371	0·258	0·371
5		0·372	0·256	0·372	0·379	0·243	0·379

orthohexagonal **b** vector during one period. In accordance with this the value $\pi'(1,1)$–$\pi'(-1,1)$ gives the 'relative cyclicity' of a faulted lattice. In the case of symmetrical fault distribution, *i.e.* if the occurrence rate of an individual structure element does not change when replacing the 1's by 0's and *vice versa,* this cyclicity value is equal to zero. This corresponds to equal probability of lattice shifts in the directions **b** and $-\mathbf{b}$. In this case the diffraction patterns of crystals with both periodically and non-periodically stacked lattices are symmetrical about the equator. It has to be mentioned that in the majority of the cases we obtain such patterns from stacking-faulted crystals.

Also the rate of occurrence of two-layer structure elements can be completely determined using the calculated $\pi'(m,2)$ values. As in the case of periodic polytypes

$$\begin{aligned}\pi'(-1,2)&=[11]'\\ \pi'(1,2)\quad&=[00]'\end{aligned}\qquad(5)$$

and

$$\pi'(0,2)=[10]'+[01]'=2[10]'.\qquad(6)$$

This means that the relative rate of occurrence of the two cubic sequences, '11' and '00' and of the two hexagonal sequences, '10' and '01' may be directly calculated. The quantity $[10]'+[01]'$ is the so-called 'percentage of hexagonality', α, also widely used to characterize polytypes of faulted structures (Brafman & Steinberger, 1966; Nelkowski & Pfützenreuter, 1971).

As demonstrated, our method is suitable for deriving α from the measured intensity data by calculating $\pi'(0,2)$ in the above-mentioned way.

Already, the possibility of direct determination of hexagonality is very useful in practice, *i.e.* when trying to find correlation between structure and some physical properties of faulted crystals. However, our method offers a more advantageous possibility: the direct determination of the relative rate of occurrence of structure elements built up of four layers (three subsequent stackings) could be achieved.

Using the recursion formulae derived originally for periodic polytypes (Dornberger-Schiff & Farkas-Jahnke, 1970), in a somewhat modified form, the connexion between the relative rate of occurrence for sequences of lengths 2 and 3 is obtained:

$$\begin{aligned}[a_1\ a_2]'&=[a_1\ a_2\ 0]'+[a_1\ a_2\ 1]'\\ [a_1\ a_2]'&=[0\ a_1\ a_2]'+[1\ a_1\ a_2]'\end{aligned}\qquad(7)$$

(here a_1 denotes 1 or 0 and $[a_1 \ldots a_p]'=[a_1 \ldots a_p]/N$). Using these equations, together with relations (5) and (6) between the $\pi'(m,2)$ and $[a_1\ a_2]'$ values and between $\pi'(m,3)$ and $[a_1\ a_2\ a_3]'$ values:

$$\begin{aligned}[000]'+[111]'&=\pi'(0,3)\\ [001]'+[010]'+[100]'&=\pi'(-1,3)\\ [011]'+[101]'+[110]'&=\pi'(1,3)\,,\end{aligned}\qquad(8)$$

it is easy to derive the equations for the $[a_1\ a_2\ a_3]'$ values. These formulae are given in Table 2.

Table 2. *Formulae for* $[\gamma]_3'$ *values*

$[000]'=\pi'(1,2)+\frac{1}{2}\pi'(0,2)-\frac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]$
$[001]'=\frac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]-\frac{1}{2}\pi'(0,2)$
$[010]'=\pi'(0,2)-\frac{1}{3}[2\pi'(1,3)+\pi'(-1,3)]$
$[011]'=\frac{1}{3}[2\pi'(1,3)+\pi'(-1,3)]-\frac{1}{2}\pi'(0,2)$
$[100]'=[001]'$
$[101]'=\pi'(0,2)-\frac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]$
$[110]'=[011]'$
$[111]'=\pi'(-1,2)+\frac{1}{2}\pi'(0,2)-\frac{1}{3}[2\pi'(1,3)+\pi'(-1,3)]$

Thus by using the experimental data it is possible to determine directly not only the hexagonality value of the structure but also the relative rate of occurrence of four layers stacked in the cubic sense and even the relative rate of occurrence of all possible four-layer stackings.

The connexion between the fault parameters α and β used by Jagodzinski and the rate of occurrence of three and four-layer stackings

At this point in discussing the suitability of our method for the determination of stacking-fault probabilities in the ZnS structure (and in all structures built up of translationally equivalent layers) we have to show that by determining $[\gamma]_2'$ and $[\gamma]_3'$ in a direct way we obtain the same result in characterizing the faulted structure as is achieved by the most frequently used indirect methods, for example the method of Jagodzinski.

For this purpose we deduce the connexion between $[\gamma]_p'$ and $\pi'(m,p)$ values used in our method and the fault parameters α and β used by Jagodzinski (1949*a*, *b*, *c*).

According to Jagodzinski, the hexagonal stackings of three subsequent layers – 10 or 01 in our notation – are denoted by h, and the cubic stackings – 11 or 00 – by k. The probability that a fourth layer will be stacked in a cubic sense following a hexagonal stacking is denoted by α, and when following a cubic stacking by β. Thus the probability of two subsequent hexagonal stackings is $(1-\alpha)$, and that of a hexagonal one after a cubic stacking is $(1-\beta)$ (see Fig. 4). (We should mention that the fault parameter α used by Jagodzinski is different from that used for denoting hexagonality by other authors.)

Denoting by $[h]'$ and $[k]'$ the probabilities (*i.e.* the relative rates of occurrence) of hexagonal and cubic stack-

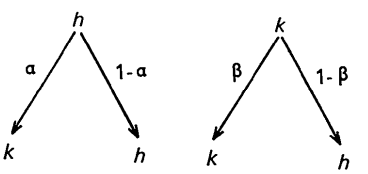


Fig. 4. Probability of the possible four-layer stackings according to Jagodzinski.

ings, respectively, in the structure, we may write the following equations:

$$[h]' = [01]' + [10]' = 2\,[01]' = \pi'(0,2)$$

and

$$[k]' = [00]' + [11]'. \tag{10}$$

The equation

$$[h]' + [k]' = 1 \tag{11}$$

is obviously satisfied.

For the probabilities of four-layer stackings the following equations are valid

$$[hh]' = [h]'\,(1-\alpha) = [010)' + [101]' \tag{12a}$$

$$[hk]' = [h]'\,\alpha \quad = [011]' + [100]' \tag{12b}$$

$$[kh]' = [k]'\,(1-\beta) = [001]' + [110]' \tag{12c}$$

$$[kk]' = [k]'\,\beta = (1-[h]')\,\beta = [000]' + [111]' = \pi'(0,3)\,. \tag{12d}$$

From equation (12*d*) we get

$$\beta = \frac{\pi'(0,3)}{1-\pi'(0,2)}\,. \tag{13}$$

If the three-layer stackings are followed by a fourth layer, the following recursion formulae are valid for their relative rates of occurrence:

$$[01]' = [010]' + [011]' \tag{14a}$$

$$[01]' = [001]' + [101]' \tag{14b}$$

and

$$[10]' = [100]' + [101]' \tag{15a}$$

$$[10]' = [010]' + [110]'. \tag{15b}$$

Since $[10]' = [01]'$, from (14*b*) and (15*a*) it follows, that

$$[100]' = [001]'$$

and from (14*a*) and (15*b*) that

$$[011]' = [110]'.$$

Using these results we obtain from (12*b*) and (12*c*):

$$[h]'\alpha = [k]'\,(1-\beta) = (1-[h]')\,.\,(1-\beta)\,, \tag{16}$$

and with formula (13),

$$\alpha = \frac{1-\pi'(0,2)-\pi'(0,3)}{\pi'(0,2)}\,. \tag{17}$$

Consequently, by using our method it is possible to determine, if desired, the parameters α and β by a very simple calculation, and by using these parameters to obtain the best fitting Jagodzinski-type curve.

This fact can be useful for determining whether the approximation used in our method when replacing $|S(0,1,l)|^2$ in equation (3) by the values derived from intensities at discrete points in the continuous distributions is allowable. Intensity distributions were calculated according to the formulae of Jagodzinski for various α and β parameter pairs. Using a value of 48 for N, $\pi'(m,p)$ sets were calculated according to equation (3), and from these α' and β' values were derived by equations (13) and (17). The difference between the starting and final values of α and β was in all cases less than 2%. Some of these α and β pairs are given in Table 3.

This little experiment proved two things: firstly that our method of approximating $|S(h,k,l)|^2$ values of the discrete reflexions by those calculated from the blackening of the continuous diffuse lines at adequate points is allowable, and the error caused by that approxima-

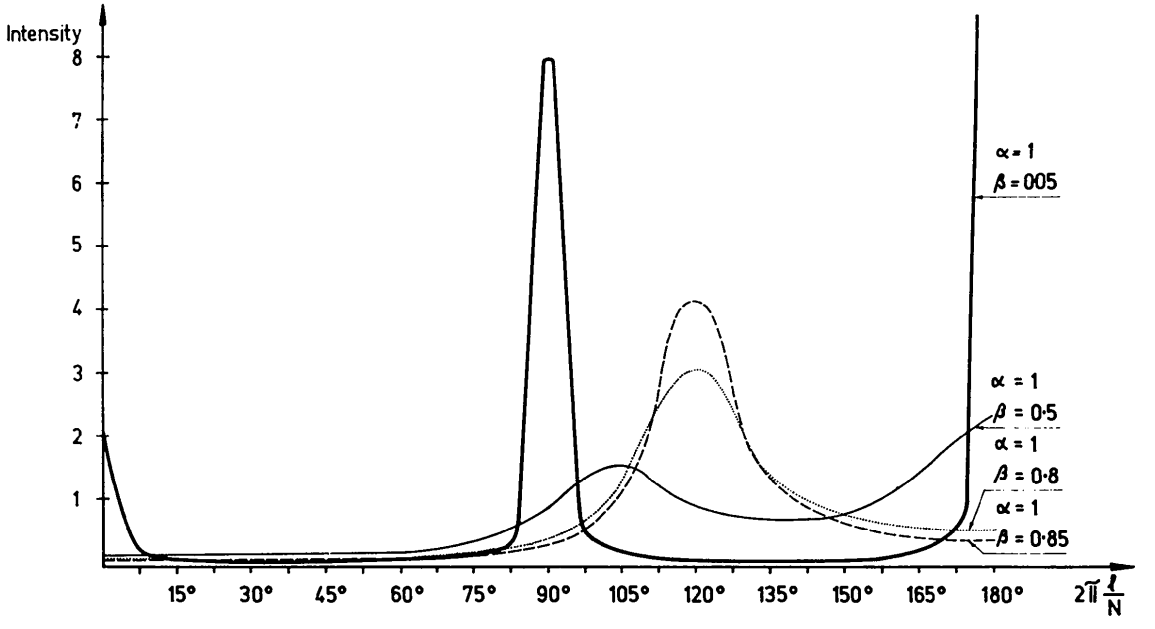


Fig. 5. Some characteristic intensity distribution curves, calculated along the 01*l* line of the reciprocal space according to the theory of Jagodzinski.

Table 3. *Starting and final values of fault parameters α and β*

Values of α and β				Maximal error
Starting		Calculated		
α	β	α	β	%
0·15	0·65	0·1500	0·6498	0·20
0·30	0·45	0·2999	0·4500	0·04
0·75	0·25	0·7497	0·2497	0·12
0·95	0·50	0·9500	0·4999	0·02

tion is certainly not larger than that of the calculated α and β values.

Secondly, we got back in all cases as parameters of the best fitting curve the starting α and β values (within the limits of the error), *i.e.* the starting intensity distributions. Thus we may conclude that by using our method it is possible to determine the α and β parameters of the best fitting Jagodzinski-curve for any measured intensity distribution.

It also allows the possibility of demonstrating the limits of Jagodzinski's method in practice. As mentioned in his papers Jagodzinski (1949*a*,*b*,*c*) takes into consideration when determining the intensity distribution formula only interactions of 'Reichweite' = 3, *i.e.* interactions between layers separated by more than four interlayer spacings are neglected. Consequently, curves calculated with the aid of his formula are rather smooth, as shown for some special cases in Fig. 5, unlike most experimental curves. This is probably the reason why the fitting of experimental curves to the Jagodzinski-type master curves succeeded only in a few special cases (Müller, 1952; Singer & Gashurov, 1963).

In Fig. 6, three intensity distribution curves measured along the enclosed X-ray oscillation patterns are given, together with their best fitting Jagodzinski-curves. The α and β parameters for these were determined using equations (13) and (17) by the method described above. The Figures show that adequate fitting was obtained in case (*a*) only, where the investigated structure was a faulted hexagonal one. In case (*b*), where the investigated region contains, besides the faulted cubic, a faulted 6*H* structure as well, the Jagodzinski-curve describes the two cubic-type maxima, but none of the 6*H* peaks. In the third case, where the pattern was made of a faulted polytype structure of long periodicity (where interactions between layers at a distance apart greater than 4 interlayer spacings are present) even the best fitting Jagodzinski-curve fails in following the greatest maxima of the real intensity distribution.

Conclusions

Unlike numerous authors who have made great efforts to characterize various stacking-faulted structures using indirect methods, we chose a direct way for solving the problem. As we have shown above, the method used for the determination of the structure of periodic polytypes might also be succesfully applied in a slightly modified form for determining characteristics of faulted, non-periodic stackings.

Using this method it is possible to calculate directly from the measured intensity distribution of diffuse lines along row-lines $h-k \neq 3n$ the relative rate of occurrence of stacking vectors, and from these values the cyclicity, hexagonality and the relative rate of occurrence of the various four-layer stackings in the investigated region of the lattice. From these values the fault parameters required for indirect methods might also be derived, if necessary. The maximum error in the determination is not more than 1 %.

The possibility of determining of the relative rate of occurrence of different structure elements has useful practical applications. For example, with the aid of this method it is possible to explain the results of some physical experiments, *i.e.* to find the relation between certain physical properties and the structure of the faulted crystals, and further to reveal the range of interaction influencing the property investigated.

Another interesting area of application is the investigation of the changes in the structure due to heat treatment or mechanical deformation. By recording a set of diffraction patterns during the course of such processes the mode of transformation may be determined. Results of investigations of both these possibilities will be published shortly.

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A New Direct Method for Characterizing Structures with Stacking Faults, Built up from Translationally Equivalent Layers. II. Faults in Five-Layer Structure Elements

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A method is given for calculating fault parameters in lattices built up of translationally equivalent layers with interactions between five subsequent layers, *i.e.* the relative rate of occurrence of five-layer structure elements in such lattices. Based on a method outlined in part I, formulae are derived for the determination of these characteristic values from the data of X-ray patterns with symmetrical or asymmetrical intensity distribution. The validity of the method is tested on model structures.

In part I of the present work (Farkas-Jahnke, 1973) a method was described for the determination of fault parameters, or more precisely relative rates of occurrence of structure elements in lattices, where the planes lying perpendicular to one crystallographic axis can be transferred into each other by one translation. From the intensities of diffuse lines along row lines whose Miller indices satisfy the inequality $h-k\neq 3n$, the rate of occurrence of structure elements consisting of three or four subsequent layers, $[\gamma]'_2$ or $[\gamma]'_3$, can be determined by using a direct method.

Even by using these fault parameters a number of practical problems can be solved, for example in cases where the investigated physical property of the material depends on the hexagonality or on the relative rate of four-layer cubic stackings in the lattice, but for many other practical applications the determination of fault parameters taking into account interactions between layers at greater distances would be desirable. Such a problem is the investigation of the course of phase transformations either during heat treatment (Farkas-Jahnke, 1971) or due to mechanical forces. Even the determination of the range of interaction in lattices would be possible by the determination of rate of occurrences of longer structure elements (Dornberger-Schiff, 1972).

Because of the difficulties outlined in the next section, the determination process is somewhat difficult even for five-layer elements. In the present paper we give a solution of the problem; the concept applied can be extended later to determine fault parameters in longer structure elements.

The calculation of $[\gamma]'_p$ values for $p>3$

As we have shown in the case of periodic polytypes, $[\gamma]'_p$ values, *i.e.* relative rates of occurrences of structure elements consisting of $p+1$ layers can be derived for any p using the recursion formulae and the equations valid between $\pi(m,p)$ and $[\gamma]_p$ values (Dornberger-Schiff & Farkas-Jahnke, 1970). In this case, however, the values of the Patterson-like function, $\pi(m,p)$ and $[\gamma]_p$, could only be integers, according to their definition. Although the number of equations is less than that of the unknown $[\gamma]_p$'s, the integer nature of the quantities yielded a possibility of determining $[\gamma]_p$ values even for $p>3$, if the measurement of the intensities were accurate enough.

Up to $p=3$ it was not necessary, however, to make use of the integer nature of these quantities. The number of equations (the recursion formulae and the relations between $\pi(m,p)$ and $[\gamma]_p$ values together) is large enough to allow us to calculate $[\gamma]_2$ and $[\gamma]_3$ sets directly. As we have already shown (Farkas-Jahnke, 1973), up to this step the $[\gamma]'_p=[\gamma]_p/N$ values can also be calculated directly (Table 2 in part I), the same type of equations being valid for this case as for periodic polytypes. But as we have seen these $[\gamma]'_p$'s are no longer integers;