LELE, S., ANANTHARAMAN, T. R. & JOHNSON, C. A. (1967). *Phys. Stat. Sol.* **20**, 59–68.
LELE, S., PRASAD, S. & ANANTHARAMAN, T. R. (1969). *Acta Cryst.* A**25**, 471–475.
LELE, S. & RAMA RAO, P. (1970). *Scripta Metall.* **4**, 43–50.
MÜLLER, H. (1952). *Neues Jb. Miner. Mh.* **84**, 43–76.
NELKOWSKI, H. & PFÜTZENREUTER, O. (1971). *Acta Cryst.* A**27**, 296–298.
PATERSON, M. S. (1952). *J. Appl. Phys.* **23**, 805–811.
PRASAD, B. & LELE, S. (1971). *Acta Cryst.* A**27**, 54–64.
SATO, R. (1966). *Acta Cryst.* **20**, 150–151.
SATO, R. (1969). *Acta Cryst.* A**25**, 309–318.
SHACHAR, G., MARDIX, S. & STEINBERGER, I. T. (1968). *J. Appl. Phys.* **39**, 2485–2486.
SINGER, J. & GASHUROV, G. (1963). *Acta Cryst.* **16**, 601–604.
VERMA, A. R. & KRISHNA, P. (1966). *Polymorphism and Polytypism in Crystals.* New York: John Wiley.
WARREN, B. (1941). *Phys. Rev.* **59**, 693–698.
WILSON, A. J. C. (1942). *Proc. Roy. Soc.* A**180**, 277–285.

Acta Cryst. (1973). B**29**, 413

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;

their values, like the $\pi'(m,p)$ values, are less than unity. Since the number of equations was not enough to demine the $[\gamma]'_p$ values for $p>3$, we had to evaluate a method of overcoming this difficulty.

Relations between $[\gamma]'_4$ values

From the recursion formulae there are relations between $[\gamma]'_3$ and $[\gamma]'_4$ values. This enables us to reduce the number of unknown $[\gamma]'_4$ quantities from 16 to 4, as shown in the first column in Table 1.

Table 1. *Relations between $[\gamma]'_4$ and $[\gamma]'_3$ values according to the recursion formulae*

Asymmetrical $\pi'(m,p)$ set	Symmetrical $\pi'(m,p)$ set
$[0]'_4=[0]'_3-[1]'_4$	$[0]'_4=[0]'_3-[1]'_4$
$[1]'_4=[1]'_4$	$[1]'_4=[1]'_4$
$[2]'_4=[2]'_4$	$[2]'_4=[2]'_4$
$[3]'_4=[1]'_3-[2]'_4$	$[3]'_4=[1]'_3-[2]'_4$
$[4]'_4=[4]'_4$	$[4]'_4=[4]'_4$
$[5]'_4=[2]'_3-[4]'_4$	$[5]'_4=[2]'_3-[4]'_4$
$[6]'_4=[3]'_3-[7]'_4$	$[6]'_4=[1]'_3-[1]'_4$
$[7]'_4=[7]'_4$	$[7]'_4=[1]'_4$
$[8]'_4=[1]'_4$	$[8]'_4=[1]'_4$
$[9]'_4=[1]'_3-[1]'_4$	$[9]'_4=[1]'_3-[1]'_4$
$[10]'_4=[2]'_3-[2]'_4$	$[10]'_4=[2]'_3-[2]'_4$
$[11]'_4=[3]'_3-[1]'_3+[2]'_4$	$[11]'_4=[2]'_4$
$[12]'_4=[4]'_3-[4]'_4=[1]'_3-[4]'_4$	$[12]'_4=[1]'_3-[4]'_4$
$[13]'_4=[5]'_3-[2]'_3+[4]'_4$	$[13]'_4=[4]'_4$
$[14]'_4=[7]'_4$	$[14]'_4=[1]'_4$
$[15]'_4=[7]'_3-[7]'_4$	$[15]'_4=[0]'_3-[1]'_4$

(Note: In the following we shall abbreviate the binaries to their decimal equivalent form, as we have done when dealing with the structure determination of periodic polytypes. So, we shall write for example $[0]'_4$ for $[0000]'$ and $[4]'_4$ for $[0100]'$.)

It is clear from Table 1 that the $[\gamma]'_4$ values may be devided into two groups: $[0]'$, $[6]'$, $[7]'$, $[8]'$, $[9]'$, $[14]'$, $[15]'$ are related to $[1]'$ (and $[7]'$) and $[3]'$, $[5]'$, $[10]'$, $[11]'$, $[12]'$, $[13]'$ to $[2]'$, and $[4]'$ only. These two groups of unknown $[\gamma]'_4$'s will be referred to in the following as the 'first group' and the 'second group' of $[\gamma]'_4$.

As with the equations I(8) (equation 8 of part I), giving the connexion between $[\gamma]'_3$ and $\pi'(m,3)$ values, it is possible to write the same types of equation for $p=4$, as follows:

$$[0]'_4+2[7]'_4+[11]'_4+[13]'_4=\pi'(-1,4) \qquad (1a)$$

$$2[1]'_4+[2]'_4+[4]'_4+[15]'_4=\pi'(1,4) \qquad (1b)$$

$$[3]'_4+[5]'_4+[6]'_4+[9]'_4+[10]'_4+[12]'_4=\pi'(0,4)\,. \qquad (1c)$$

(Remember that according to the recursion formulae $[7]'_4=[14]'_4$, and $[1]'_4=[8]'_4$.)

To reduce further the number of unknown $[\gamma]'_4$ values, we use the relations between them given in Table 1 and substitute them into (1*a*), (1*b*) and (1*c*). They are now in the following form (using also Table 2 in part I):

$$2[7]'_4-[1]'_4+[2]'_4+[4]'_4=\pi'(-1,4)+\pi'(-1,3)-\pi'(1,2) -\tfrac{1}{2}\pi'(0,2)-\tfrac{1}{3}[\pi'(1,3)-\pi'(-1,3)] \qquad (2a)$$

$$2[1]'_4+[2]'_4+[4]'_4-[7]'_4=\pi'(1,4)+\pi'(1,3)-\pi'(-1,2) -\tfrac{1}{2}\pi'(0,2)-\tfrac{1}{3}[\pi'(1,3)-\pi'(-1,3)] \qquad (2b)$$

$$[1]'_4+2[2]'_4+[7]'_4+2[4]'_4=\pi'(1,3)+\pi'(-1,3)-\tfrac{2}{3}[\pi'(1,3) -\pi'(-1,3)]-\pi'(0,4)\,. \qquad (2c)$$

Solving this system of equations two relations are obtained:

$$[7]'_4=[1]'_4-\tfrac{1}{3}[\pi'(1,4)-\pi'(-1,4)]-\tfrac{1}{3}[\pi'(1,3) -\pi'(-1,3)]-\tfrac{1}{3}[\pi'(1,2)-\pi'(-1,2)] \qquad (3a)$$

and

$$[2]'_4+[4]'_4=\tfrac{1}{3}\{[2\pi'(1,4)+\pi'(-1,4)]+[2\pi'(-1,3) +\pi'(1,3)]-[\pi'(1,2)+2\pi'(-1,2)]\}-\tfrac{1}{2}\pi'(0,2)-[1]'_4\,. \qquad (3b)$$

Having made use of our equations, in Table 2 we list the formulae gained so far for the determination of the $[\gamma]'_4$ values. It is clear that the $[\gamma]'_4$ values are still dependent on at least two unknown quantities. Therefore a procedure was sought to overcome this difficulty.

Determination of $[\gamma]'_4$ values from symmetrical $\pi'(m,p)$ sets

If the intensity distributions along row-lines of oscillation X-ray patterns with Miller indices $(h-k)\neq 3n$ are

Table 2. *Formulae for determination of non-symmetrical $[\gamma]'_4$ values*

$$[0]'_4=\pi'(1,2)+\tfrac{1}{2}\pi'(0,2)-\tfrac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]-[1]'_4$$
$$[1]'_4=[1]'_4$$
$$[2]'_4=[2]'_4$$
$$[3]'_4=\tfrac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]-\tfrac{1}{2}\pi'(0,2)-[2]'_4$$
$$[4]'_4=\tfrac{1}{3}[(2\pi'(1,4)+\pi'(-1,4))+(2\pi'(-1,3)+\pi'(1,3))-(\pi'(1,2)+2\pi'(-1,2))]-\tfrac{1}{2}\pi'(0,2)-[1]'_4-[2]'_4$$
$$[5]'_4=\tfrac{3}{2}\pi'(0,2)-\tfrac{1}{3}[\pi'(-1,4)+2\pi'(1,4)]-[\pi'(1,3)+\pi'(-1,3)]+\tfrac{1}{3}[\pi'(1,2)+2\pi'(-1,2)]+[1]'_4+[2]'_4$$
$$[6]'_4=\pi'(1,3)-\tfrac{1}{2}\pi'(0,2)+\tfrac{1}{3}[\pi'(1,4)-\pi'(-1,4)+\pi'(1,2)-\pi'(-1,2)]-[1]'_4$$
$$[7]'_4=[1]'_4-\tfrac{1}{3}[\pi'(1,4)-\pi'(-1,4)+\pi'(1,3)-\pi'(-1,3)+\pi'(1,2)-\pi'(-1,2)]$$
$$[8]'_4=[1]'_4$$
$$[9]'_4=\tfrac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]-\tfrac{1}{2}\pi'(0,2)-[1]'_4$$
$$[10]'_4=\pi'(0,2)-\tfrac{1}{3}[2\pi'(1,3)+\pi'(-1,3)]-[2]'_4$$
$$[11]'_4=\tfrac{1}{3}[\pi'(1,3)-\pi'(-1,3)]+[2]'_4$$
$$[12]'_4=\tfrac{1}{3}[\pi'(1,2)+2\pi'(-1,2)]-\tfrac{1}{3}[2\pi'(1,4)+\pi'(-1,4)]+[1]'_4+[2]'_4$$
$$[13]'_4=\tfrac{1}{3}[(2\pi'(1,4)+\pi'(-1,4))+(2\pi'(1,3)+\pi'(-1,3))-(\pi'(1,2)+2\pi'(-1,2))]-\tfrac{1}{2}\pi'(0,2)-[1]'_4-[2]'_4$$
$$[14]'_4=[1]'_4-\tfrac{1}{3}[\pi'(1,4)-\pi'(-1,4)+\pi'(1,3)-\pi'(-1,3)+\pi'(1,2)-\pi'(-1,2)]$$
$$[15]'_4=\tfrac{1}{3}[\pi'(1,4)-\pi'(-1,4)]-\tfrac{1}{3}[2\pi'(-1,3)+\pi'(1,3)]+\tfrac{1}{3}[2\pi'(-1,2)+\pi'(1,2)]+\tfrac{1}{2}\pi'(0,2)-[1]'_4$$

symmetrical with respect to the equator, $\pi'(p,m)$ values calculated from these intensity values according to

$$\pi'(m,p)=\frac{1}{3}\left[1+2\sum_{l=0}^{N-1}\frac{|S(0,1,l)|^2}{N^2}\cos 2\pi\cdot\left(\frac{m}{3}+l\frac{p}{N}\right)\right] \quad \text{I(3)}$$

will be symmetrical in m, *i.e.* $\pi'(m,p)=\pi'(-m,p)$ for any p value. It is clear that in this case equations (2) become more simple, and from (3*a*) we now obtain

$$[7]'_4=[1]'_4\,. \quad (4)$$

and from (3*b*)

$$[1]'_4+[2]'_4+[4]'_4=\pi'(1,4)-\frac{\pi'(0,3)}{2}\,. \quad (5)$$

[Note: Since the equation $\sum_m \pi'(m,p)=1$ holds in general, for symmetrical $\pi'(m,p)$ sets the relation

$$\pi'(-1,p)+\tfrac{1}{2}\pi'(0,\,p)=\tfrac{1}{2}$$

is valid. From this it follows that:

$$\pi'(1,p_i)-\frac{\pi'(0,p_k)}{2}=\pi'(1,p_k)-\frac{\pi'(0,p_i)}{2}\,.\;]$$

Although the form of the equations for the determination of $[\gamma]'_4$ values becomes more simple, as shown in the second column of Table 1, we did not essentially get any further, since the number of unknown quantities did not decrease. To overcome our difficulties, we have to consider a moderately large group of the faulte structures.

Structure elements derived from each other by replacing 1's by 0's and *vice versa* in their binary notation, should be called related structure elements.

We tried to find a solution for structures where the relative rates of occurrence of related structure elements are equal.

This will certainly be valid for a number of structures, since it only means that the probability of a fault caused by a slip of the lattice to the right is equal to the probability of a fault caused by the same slip in the opposite direction.

So, for example, in the symmetrical case

$$[0010]'=[1101]'$$

i.e.

$$[2]'_4 \text{ symmetrical}=[13]'_{4s}=[4]'_{4s} \text{ (see Table 1).} \quad (6)$$

Hereafter if relations of type (6) are valid between corresponding pairs of a $[\gamma]'_4$ set, they will be termed symmetrical, and denoted by an 's' in their index, *i.e.* $[\gamma]'_{4s}$ is one of a set of $[\gamma]'_4$ values where the relative rates of related structure elements is equal.

From equation (5) and using equation (6) a relation between $[2]'_{4s}$ and $[1]'_{4s}$ may be derived:

$$[2]'_{4s}=\tfrac{1}{2}\left[\pi'(1,4)-\frac{\pi'(0,3)}{2}\right]-[1]'_{4s} \quad (7)$$

and so the relations in Table 2 may be transformed into formulae, where all $[\gamma]'_{4s}$ values depend on just one unknown quantity, $[1]'_{4s}$. These relations are listed in Table 3.

Table 3. $[\gamma]'_{4s}$ *values*

$$[0]'_{4s}=\tfrac{1}{2}\pi'(0,3)-[1]'_{4s}$$
$$[1]'_{4s}=[1]'_{4s}$$
$$[2]'_{4s}=\tfrac{1}{2}\pi'(1,4)-\tfrac{1}{4}\pi'(0,3)-\tfrac{1}{2}[1]'_{4s}$$
$$[3]'_{4s}=\pi'(1,2)-\tfrac{1}{4}\pi'(0,3)-\tfrac{1}{2}\pi'(1,4)+\tfrac{1}{2}[1]'_{4s}$$
$$[4]'_{4s}=[2]'_{4s}$$
$$[5]'_{4s}=\pi'(0,2)-\tfrac{3}{2}\pi'(1,3)+\tfrac{1}{4}\pi'(0,4)+\tfrac{1}{2}[1]'_{4s}$$
$$[6]'_{4s}=\pi'(1,2)-\tfrac{1}{2}\pi'(0,3)-[1]'_{4s}$$
$$[7]'_{4s}=[1]'_{4s}$$

The number of unknown quantities on the right hand side of the equations now decreases to one. So, although it is still not possible to determine exactly the values of the $[\gamma]'_{4s}$'s, it is at least possible to indicate their maximum and minimum values as given in Table 4. {The limits of the unknown quantities are given by the recursion formulae

$$[a_1a_2\ldots a_p]=[a_1a_2\ldots a_p0]+[a_1a_2\ldots a_p1]$$
$$[a_1a_2\ldots a_p]=[0a_1a_2\ldots a_p]+[1a_1a_2\ldots a_p]$$

where a_1 denotes 1 or 0 [Dornberger-Schiff & Farkas-Jahnke, 1970, Table 3(*b*)], and by the relations between $\pi(m,p)$ values and the sum of rate of occurrences of structure elements with digital sum, $K=3-p-m$ (mod 3). For example see equations (7) and (8) in part I, or Table 1 and equation (1*a*,*b*,*c*) in this work}.

Values lying within the intervals allowed for each $[\gamma]'_4$ give the possible solutions of the problem. If we choose for any of the unknown quantities a value of its allowed interval, a set of $[\gamma]'_4$ values, all lying within their allowed interval, follows. Changing the value of the chosen unknown (for example that of $[1]'_4$) linearly, the values of the other $[\gamma]'_4$ quantities also change linearly. This means, if we choose for $[\gamma]'_{4s}$ the mean value of $[1]'_{4s\,\max}$ and $[1]'_{4s\,\min}$, *i.e.* the middle point of its allowed interval, the $[\gamma]'_{4sm}$ set derived using this $[1]'_{s4}$ mean consists of the middle points of each $[\gamma]'_{4s}$ interval.

$$[\gamma]'_{4sm}=\frac{[\gamma]'_{4s\,\max}+[\gamma]'_{4s\,\min}}{2}\,.$$

With the described procedure we obtain a $[\gamma]'_4$ set which may be regarded as a probable solution of our problem.

In the following we shall characterize the structures with 'symmetrical' stacking faults by these mean $[\gamma]'_{4\,sm}$ values.

It is clear that this set of mean values will be the more characteristic of the structure the shorter the intervals for the allowed $[\gamma]'_{4s}$ values, and the greater the accuracy of measurement of intensity values on the X-ray pattern. In practice it quite often happens that the calculation of the minimum of one or other $[\gamma]'_4$ yields a negative value. Since according to their definition the $[\gamma]'_4$'s can have only positive values, this calculated limit should be increased to 0, and the values of all other $[\gamma]'_{4s}$ have to be changed appropriately. This correction certainly shortens the interval, and allows the possibility of increasing the accuracy in approaching the real fault parameters when replacing them by the mean values of the $[\gamma]'_4$ intervals.

Thus we have solved our problem for the simplest case when

(1) the $\pi'(m,p)$ sets are symmetrical in m, and
(2) the relative rates of occurrence of related structure elements are equal.

For such structures we are able to calculate characteristic parameters, which are directly derived from measured intensities and are therefore free from the errors of 'trial and error' methods.

Relation between asymmetrical $[\gamma]'_4$ and symmetrical $[\gamma]'_{4s}$ values

The considerations outlined in the third chapter resulted in equations (given in Table 2) valid between asymmetrical $[\gamma]'_4$ values. On the other hand, according to the previous section we can find a solution to the problem in a special case, starting from a symmetrical $\pi'(m,p)$ set. If we could derive a symmetrical $\pi'(m,p)$ set from the asymmetrical one we could use these results as an intermediate step in deriving the $[\gamma]'_4$ set in the asymmetrical case. This, however, can be carried out by the following procedure. It is clear that

$$\pi'(1,p)+\pi'(-1,p)+\pi'(0,p)=1$$

is generally valid, for symmetrical and also asymmetrical $\pi(m,p)$ sets. For a symmetrical set, with the same $\pi'(0,p)$ values,

$$\pi'(1,p)_s+\frac{\pi'(0,p)}{2}=\tfrac{1}{2}$$

clearly holds. From these it follows that

$$\frac{\pi'(1,p)+\pi'(-1,p)}{2}=\pi'(1,p)_s\,. \qquad (8)$$

This means that by calculating the mean value of $\pi'(1,p)$ and $\pi'(-1,p)$ a symmetrical $\pi'(m,p)$ set may be derived for each asymmetrical set. Using these symmetrized $\pi'(m,p)$ values as a starting point for the procedure sketched in the previous section, we are able to calculate a $[\gamma]'_{4sm}$ set.

Now we have to consider how to obtain relations by the aid of which it will be possible to calculate the characteristic $[\gamma]'_4$ values from this $[\gamma]'_{4s}$ set.

To derive a relation between $[1]'_4$ and $[1]'_{4s}$, which would be of greatest use to us, we have to start from equations (1*a*) or (1*b*). Then our first step must be to determine the relation between $[2]'_4+[4]'_4$ and $[2]'_{4s}$. From the recursion formulae we obtain

$$[2]'_4+[4]'_4=[11]'_4+[13]'_4-\tfrac{2}{3}[\pi'(1,3)-\pi'(-1,3)] \qquad (9)$$

Table 4. *Limits of symmetrical* $[\gamma]'_{4s}$ *values*

Valid if $\pi'(1,4)<\pi'(1,2)$

$\frac{1}{2}\pi'(0,3)$	>	$[0]'_{4s}$	>	$\pi'(0,3)-\pi'(1,4)$
0	<	$[1]'_{4s}$	<	$\pi'(1,4)-\frac{1}{2}\pi'(0,3)$
$\frac{1}{2}\pi'(1,4)-\frac{1}{4}\pi'(0,3)$	>	$[2]'_{4s}$	>	0
$\pi'(1,2)-\frac{1}{2}\pi'(1,4)-\frac{1}{4}\pi'(0,3)$	<	$[3]'_{4s}$	<	$\pi'(1,2)-\frac{1}{2}\pi'(0,3)$
$[2]'_{4s\,max}$	>	$[4]'_{4s}$	>	$[2]'_{4s\,min}$
$\pi'(0,2)-\frac{3}{2}\pi'(1,3)+\frac{1}{4}\pi'(0,4)$	<	$[5]'_{4s}$	<	$\pi'(0,2)-\pi'(1,3)$
$\pi'(1,2)-\frac{1}{2}\pi'(0,3)$	>	$[6]'_{4s}$	>	$\pi'(1,2)-\pi'(1,4)$
$[1]'_{4s\,min}$	<	$[7]'_{4s}$	<	$[1]'_{4s\,max}$

Valid if $\pi'(1,2)<\pi'(1,4)$

$\frac{1}{2}\pi'(0,3)$	>	$[0]'_{4s}$	>	$\pi'(0,3)-\pi'(1,2)$
0	<	$[1]'_{4s}$	<	$\pi'(1,2)-\frac{1}{2}\pi'(0,3)$
$\frac{1}{2}\pi'(1,4)-\frac{1}{4}\pi'(0,3)$	>	$[2]'_{4s}$	>	$\frac{1}{2}[\pi'(1,4)-\pi'(1,2)]$
$\pi'(1,2)-\frac{1}{2}\pi'(1,4)-\frac{1}{4}\pi'(0,3)$	<	$[3]'_{4s}$	<	$\frac{1}{2}[3\pi'(1,2)-\pi'(0,3)-\pi'(1,4)]$
$[2]'_{4s\,max}$	>	$[4]'_{4s}$	>	$[2]'_{4s\,min}$
$\pi'(0,2)-\frac{3}{2}\pi'(1,3)+\frac{1}{4}\pi'(0,4)$	<	$[5]'_{4s}$	<	$\frac{1}{2}\pi'(0,2)-\pi'(1,3)+\frac{1}{4}[\pi'(0,2)+\pi'(0,4)]$
$\pi'(1,2)-\frac{1}{2}\pi'(0,3)$	>	$[6]'_{4s}$	>	0
$[1]'_{4s\,min}$	<	$[7]'_{4s}$	<	$[1]'_{4s\,max}$

Table 5. *Values of* $[\gamma]'_4$ *belonging to the first group in the case of asymmetrical* $\pi(m,p)$ *set*

$$[0]'_4=\tfrac{1}{2}\pi'(0,3)+\tfrac{1}{3}[\pi'(1,2)-\pi'(-1,2)]-\tfrac{1}{6}[\pi'(1,4)-\pi'(-1,4)]-[1]'_{4s}$$
$$[1]'_4=\tfrac{1}{6}[\pi'(1,4)-\pi'(-1,4)]+\tfrac{1}{6}[\pi'(1,3)-\pi'(-1,3)]+\tfrac{1}{6}[\pi'(1,2)-\pi'(-1,2)]+[1]'_{4s}$$
$$[6]'_4=\tfrac{1}{6}[\pi'(1,4)-\pi'(-1,4)]-\tfrac{1}{6}[\pi'(1,3)-\pi'(-1,3)]+\tfrac{1}{6}[\pi'(1,2)-\pi'(-1,2)]+\pi'(1,3)-\tfrac{1}{2}\pi'(0,2)-[1]'_{4s}$$
$$[7]'_4=[1]'_{4s}-\tfrac{1}{6}[\pi'(1,4)-\pi'(-1,4)]-\tfrac{1}{6}[\pi'(1,3)-\pi'(-1,3)]-\tfrac{1}{6}[\pi'(1,2)-\pi'(-1,2)]$$
$$[8]'_4=[1]'_4$$
$$[9]'_4=-\tfrac{1}{6}[\pi'(1,4)-\pi'(-1,4)]+\tfrac{1}{6}[\pi'(1,3)-\pi'(-1,3)]-\tfrac{1}{6}[\pi'(1,2)-\pi'(-1,2)]+\pi'(-1,3)-\tfrac{1}{2}\pi'(0,2)-[1]'_{4s}$$
$$[14]'_4=[7]'_4$$
$$[15]'_4=\tfrac{1}{6}[\pi'(1,4)-\pi'(-1,4)]-\tfrac{1}{3}[\pi'(1,2)-\pi'(-1,2)]+\tfrac{1}{2}\pi'(0,3)-[1]'_{4s}$$

and from the definition of the $[\gamma]'_{4s}$ value

$$[2]'_4+[13]'_4=2[2]'_{4s}$$

and

$$[4]'_4+[11]'_4=2[2]'_{4s}\,. \tag{10}$$

From these it follows that

$$[2]'_4+[4]'_4=2[2]'_{4s}-\tfrac{1}{3}[\pi'(1,3)-\pi'(-1,3)]\,. \tag{11}$$

This is the very relation required.

Using equation (11) and the relation for $[15]_4$ in Table 2, we obtain from (1*b*)

$$[1]'_4=\tfrac{1}{6}[\pi'(1,4)-\pi'(-1,4)]+\tfrac{1}{6}[\pi'(1,3)-\pi'(-1,3)] +\tfrac{1}{6}[\pi'(1,2)-\pi'(-1,2)]+[1]'_{4s}\,. \tag{12}$$

Thus all these $[\gamma]'_4$ values in Table 2, dependent only on $[1]'_{4s}$, can now be simply calculated from the already known $[1]'_{4sm}$ value using equation (12). The appropriate formulae are listed in Table 5.

For the second group of $[\gamma]'_4$ values, dependent not only on $[1]'_4$ but also on $[2]'_4$, we have to repeat the procedure used when deriving the $[\gamma]'_{4s}$ values. Either the recursion formulae or equation (11) now gives the necessary limiting conditions for these $[\gamma]'_4$ values; in a given case we have to use the one that corresponds to stricter limits, *i.e.* shorter intervals for the allowed $[\gamma]'_4$ values. Now we shall again accept as $[\gamma]'_4$ mean values the middle point of these intervals.

Since the formulae in Table 2 contain $[1]'_4$ (which is already determined at this point of the procedure) and $[2]'_4$ as unknown quantities, it seems sufficient to calculate the limits only for $[2]'_4$, and substitute the mean value of $[2]'_{4\,max}$ and $[2]'_{4\,min}$ into the formulae of the Table. But, as we have already pointed out in the previous section, it may happen that the calculated limits for one or other $[\gamma]'_4$ are less than zero. This again permits us to decrease the allowed interval for *all* $[\gamma]'_4$'s of the group, and consequently to increase the accuracy in characterizing the structure by the

Table 6. *Limits of asymmetrical $[\gamma]'_4$ values belonging to the second group*

From (*a*) and (*b*) the one corresponding to the lower value of $[2]'_{4\,max}$ is to be used.

(*a*)

0	$<$	$[2]'_4$	$<$	$\frac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]-\frac{1}{2}\pi'(0,2)$
$\frac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]-\frac{1}{2}\pi'(0,2)$	$>$	$[3]'_4$	$>$	0
$2[2]'_{4s}-\frac{1}{3}[\pi'(1,3)-\pi'(-1,3)]$	$>$	$[4]'_4$	$>$	$2[2]'_{4s}+\frac{1}{2}\pi'(0,2)-\frac{1}{3}[\pi'(-1,3)+2\pi'(1,3)]$
$\pi'(0,2)-\frac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]-2[2]'_{4s}$	$<$	$[5]'_4$	$<$	$\frac{1}{2}\pi'(0,2)-2[2]'_{4s}$
$\pi'(0,2)-\frac{1}{3}[2\pi'(1,3)+\pi'(-1,3)]$	$>$	$[10]'_4$	$>$	$\frac{3}{2}[\pi'(0,2)]-[\pi'(1,3)+\pi'(-1,3)]$
$\frac{1}{3}[\pi'(1,3)-\pi'(-1,3)]$	$<$	$[11]'_4$	$<$	$\frac{1}{3}[\pi'(-1,3)+2\pi'(1,3)]-\frac{1}{2}\pi'(0,2)$
$\frac{1}{3}[\pi'(-1,3)+2\pi'(1,3)]-\frac{1}{2}\pi'(0,2)-2[2]'_{4s}$	$<$	$[12]'_4$	$<$	$\pi'(1,3)+\pi'(-1,3)-\pi'(0,2)-2[2]'_{4s}$
$2[2]'_{4s}$	$>$	$[13]'_4$	$>$	$2[2]'_{4s}+\frac{1}{2}\pi'(0,2)-\frac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]$

(*b*)

0	$<$	$[2]'_4$	$<$	$2[2]'_{4s}-\frac{1}{3}[\pi'(1,3)-\pi'(-1,3)]$
$\frac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]-\frac{1}{2}\pi'(0,2)$	$>$	$[3]'_4$	$>$	$\frac{1}{3}[2\pi'(1,3)+\pi'(-1,3)]-\frac{1}{2}\pi'(0,2)-2[2]'_{4s}$
$2[2]'_{4s}-\frac{1}{3}[\pi'(1,3)-\pi'(-1,3)]$	$>$	$[4]'_4$	$>$	0
$\pi'(0,2)-\frac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]-2[2]'_{4s}$	$<$	$[5]'_4$	$<$	$\pi'(0,2)-\frac{1}{3}[\pi'(-1,3)+2\pi'(1,3)]$
$\pi'(0,2)-\frac{1}{3}[2\pi'(1,3)+\pi'(-1,3)]$	$>$	$[10]'_4$	$>$	$\pi'(0,2)-\frac{1}{3}[2\pi'(-1,3)+\pi'(1,3)]-2[2]'_{4s}$
$\frac{1}{3}[\pi'(1,3)-\pi'(-1,3)]$	$<$	$[11]'_4$	$<$	$2[2]'_{4s}$
$\frac{1}{3}[\pi'(-1,3)+2\pi'(1,3)]-\frac{1}{2}\pi'(0,2)-2[2]'_{4s}$	$<$	$[12]'_4$	$<$	$\frac{1}{3}[\pi'(1,3)+2\pi'(-1,3)]-\frac{1}{2}\pi'(0,2)$
$2[2]'_{4s}$	$>$	$[13]'_4$	$>$	$\frac{1}{3}[\pi'(1,3)-\pi'(-1,3)]$

Table 7. *Limits of asymmetrical $[\gamma]'_4$ values belonging to the second group, if the $\pi'(m,p)$ set is symmetrical*

From (*a*) and (*b*) the one corresponding to the lower value of $[2]'_{4\,max}$ is to be used.

(*a*)

0	$<$	$[2]'_4$	$<$	$\pi'(1,3)-\frac{1}{2}\pi'(0,2)$
$\pi'(1,3)-\frac{1}{2}\pi'(0,2)$	$>$	$[3]'_4$	$>$	0
$\pi'(1,3)-\frac{1}{2}\pi'(0,4)-[1]'_{4s}$	$>$	$[4]'_4$	$>$	$\frac{1}{2}\pi'(0,2)-\frac{1}{2}\pi'(0,4)-[1]'_{4s}$
$\pi'(0,2)+\frac{1}{2}\pi'(0,4)-2\pi'(1,3)+[1]'_{4s}$	$<$	$[5]'_4$	$<$	$\frac{1}{2}\pi'(0,2)+\frac{1}{2}\pi'(0,4)-\pi'(1,3)+[1]'_{4s}$
$\pi'(0,2)-\pi'(1,3)$	$>$	$[10]'_4$	$>$	$\frac{3}{2}\pi'(0,2)-2\pi'(1,3)$
0	$<$	$[11]'_4$	$<$	$\pi'(1,3)-\frac{1}{2}\pi'(0,2)$
$\frac{1}{2}\pi'(0,4)-\frac{1}{2}\pi'(0,2)+[1]'_{4s}$	$<$	$[12]'_4$	$<$	$\frac{1}{2}\pi'(0,4)-\pi'(0,2)+\pi'(1,3)+[1]'_{4s}$
$\pi'(1,3)-\frac{1}{2}\pi'(0,4)-[1]'_{4s}$	$>$	$[13]'_4$	$>$	$\frac{1}{2}\pi'(0,2)-\frac{1}{2}\pi'(0,4)-[1]'_{4s}$

(*b*)

0	$<$	$[2]'_4$	$<$	$\pi'(1,3)-\frac{1}{2}\pi'(0,4)-[1]'_{4s}$
$\pi'(1,3)-\frac{1}{2}\pi'(0,2)$	$>$	$[3]'_4$	$>$	$\frac{1}{2}\pi'(0,4)-\frac{1}{2}\pi'(0,2)+[1]'_{4s}$
$\pi'(1,3)-\frac{1}{2}\pi'(0,4)-[1]'_{4s}$	$>$	$[4]'_4$	$>$	0
$\pi'(0,2)+\frac{1}{2}\pi'(0,4)-2\pi'(1,3)+[1]'_{4s}$	$<$	$[5]'_4$	$<$	$\pi'(0,2)-\pi'(1,3)$
$\pi'(0,2)-\pi'(1,3)$	$>$	$[10]'_4$	$>$	$\pi'(0,2)+\frac{1}{2}\pi'(0,4)-2\pi'(1,3)+[1]'_{4s}$
0	$<$	$[11]'_4$	$<$	$\pi'(1,3)-\frac{1}{2}\pi'(0,4)-[1]'_{4s}$
$\frac{1}{2}\pi'(0,4)-\frac{1}{2}\pi'(0,2)+[1]'_{4s}$	$<$	$[12]'_4$	$<$	$\pi'(1,3)-\frac{1}{2}\pi'(0,2)$
$\pi'(1,3)-\frac{1}{2}\pi'(0,4)-[1]'_{4s}$	$>$	$[13]'_4$	$>$	0

middle value of these intervals. So in practice it is worth while to calculate the limits for all $[\gamma]_4'$ values according to Table 6 and make corrections if any of them happen to be less than zero, and to calculate the final $[\gamma]_4'$ mean values from Table 2 using the mean value of the corrected $[2]_{4\ \min}'$ and $[2]_{4\ \max}'$.

Thus we have solved our problem for the general case and are able to determine characteristic fault parameters, for any structure containing stacking faults, in a direct way from the diffracted intensity distribution measured on the X-ray pattern of the crystal.

Case of symmetrical $\pi'(m,p)$–asymmetrical $[\gamma]_4'$ sets

Having solved our problem in general, we now have to deal with one special case. In the fourth chapter where we described the procedure to be followed in the case of symmetrical $\pi'(m,p)$ sets, we had to assume the $[\gamma]_4'$ set was also symmetrical. But in reality we can not be sure about that, at least not in cases where in the parent polytype structure the cyclicity was larger than zero.

Our method outlined in the previous section for determination of the $[\gamma]_4'$ set in the case of a symmetrical $\pi'(m,p)$ set may surely also be adopted for that case. From the symmetrical nature of $\pi'(m,p)$ it follows that $\pi'(1,p)=\pi'(-1,p)$, and according to equation (11)

$$[2]_4'+[4]_4'=2[2]_{4s}' . \qquad (13)$$

From equation (5),

$$[1]_4'=\pi'(1,4)-\frac{\pi'(0,3)}{2}-2[2]_{4s}' \qquad (14)$$

and using equation (7)

$$[1]_4'=[1]_{4s}' .$$

The value of $[1]_4'$ and consequently the values of all other $[\gamma]_4'$ dependent only on $[1]_4'$ (*e.g.* $[0]_4'$, $[1]_4'$, $[6]_4'$, $[7]_4'$, $[8]_4'$, $[9]_4'$, $[14]_4'$, $[15]_4'$) are equal to the symmetrical $[\gamma]_{4s}'$ values.

Now we have to consider whether the $[\gamma]_4'$ values belonging to the second group will also be symmetrical. In equation (6) we have shown that if the $[\gamma]_4'$ set is symmetrical, $[2]_4'=[4]_4'$. It is easy to show that the converse is true: if $[2]_4'=[4]_4'$, the whole set of $[\gamma]_4'$ is symmetrical. As the $\pi'(m,p)$ set is symmetrical, it follows that the $[\gamma]_3'$ set is also symmetrical, and therefore from the recursion formulae for $[\gamma]_4'$:

$$[2]_4'=[11]_4'$$
$$[13]_4'=[4]_4'$$

and

$$[2]_4'-[4]_4'=[12]_4'-[3]_4'=[5]_4'-[10]_4' .$$

This means, if $[2]_4'=[4]_4'$, that a symmetrical set of $[\gamma]_4'$ follows from the symmetrical $\pi'(m,p)$ set.

It remains to be clarified on what conditions the equality between $[2]_4'$ and $[4]_4'$ will be satisfied. The possible limiting values for $[\gamma]_4'$ of the second group are easily derived from Table 6 assuming $\pi'(m,p)=\pi'(-m,p)$ and using equation (7), as seen in Table 7. Again, as in the case of Table 6, either the second or the third column of equations is valid, together with the first, depending on which of them gives the stricter limit for $[2]_{4\ \max}'$.

The $[\gamma]_4'$ values of this group can be calculated in a manner similar to the procedure followed in the case of asymmetrical $\pi'(m,p)$ sets, *i.e.* as mean values of $[\gamma]_{4\ \max}'$ and $[\gamma]_{4\ \min}'$.

From Table 7 it is obvious that using this definition for $[\gamma]_4'$ the set may be symmetrical only if the actual upper limit of $[2]_4'$ is given by column (*b*) of the Table. In this case the condition $[2]_4'=[4]_4$ is satisfied, whereas if the limiting condition is given by column (*a*) it is not.

Table 8. *Polytype models with $\pi'(m,p)$ values*

(*a*) A 48-layer polytype model

111010000101111011100101110111110011010011101101

(*b*) A 96-layer model made from the above 48-layer stacking introducing one fault between two 48-layer regions:

111010000101111011100101110111110011010011101100
111010000101111011100101110111110011010011101111

(*c*) $\pi'(m,p)$ values corresponding to the above stackings

	a			*b*		
p \ *m*	−1	0	+1	−1	0	+1
1	0·375	0	0·625	0·375	0	0·625
2	0·375	0·5	0·125	0·385	0·48	0·135
3	0·25	0·25	0·5	0·27	0·27	0·47
4	0·52	0·27	0·21	0·48	0·29	0·23

(*d*) $\pi'(m,p)$ values calculated from the artificially faulted structures based on stacking

	a			*b*		
p \ *m*	−1	0	+1	−1	0	+1
1	0·42	−0·02	0·60	0·43	−0·02	0·59
2	0·32	0·53	0·15	0·31	0·52	0·17
3	0·30	0·20	0·50	0·34	0·23	0·43
4	0·48	0·36	0·16	0·41	0·37	0·22

This condition may be given in the form of two inequalities: $[2]'_{4\ \text{mean}}=[4]'_{4\ \text{mean}}$, if

$$\pi'(1,4)+\tfrac{1}{4}\pi'(0,3)-\tfrac{1}{2}\pi'(1,2)<\pi'(1,2)<\pi'(1,4)\ ,$$

or

$$\tfrac{1}{2}\pi'(1,4)+\tfrac{1}{4}\pi'(0,3)<\pi'(1,2)>\pi'(1,4)\ .$$

Test of the validity of the method

The direct method for characterizing structures containing stacking faults works with some assumptions which seemed to be justified; nevertheless it would be desirable to estimate the errors induced by them.

It is not possible to test the validity of the method on a real structure, since it goes without saying that the real fault parameters of the structure are not known. In the fifth section of part I (Farkas-Jahnke, 1973) we have shown that the $[\gamma]'_3$ values deduced by our method are equal to those obtained by using one of the indirect methods, *i.e.* that of Jagodzinski.

For $p=4$ such comparison is not yet possible, and we therefore tried our method on an artificially made structure according to the following: structure models of pure polytypes were made by determining their stacking sequence by throwing dice. The period lengths of the stackings were 24, 48 and 96 in one group of models and 102 in others. In the latter case the three models have structures independent of each other; in the first case each group was based on a 24-layer structure. The 48-layer structure was built up from two 24-layer regions of the same stacking with one stacking fault between them, and the 96-layer structure was built up similarly from 48-layer regions. Intensities of reflexions (*i.e.* structure-factor squared values) with Miller indices $01l$ were calculated for these models according to the classical formula.

In this way we obtained a set of calculated intensities for each artificially made model structure. Since the models were pure polytypes, the intensities were different from zero only at discrete points on the $01l$ row-line. Next we connected these intensity maxima by a continuous line, thus drawing a model for the intensity distribution that would be diffracted from a lattice, which, although faulted, was based on the polytype structure of the initial model.

To arrive closer at the real situation we made a further correction. In practice, if we record an X-ray pattern from a region of a real crystal (for this purpose we use an X-ray beam some 0·1 mm wide) even the reflexions from a pure polytype lattice will be of definite breadth. Therefore we represented the intensity maxima by Gaussian curves, whose centre was placed at the site of the reflexion and whose height at that point was equal to the value of the calculated intensity. The breadths of the Gaussians were determined by measuring the width of the intensity distributions of family reflexions (*i.e.* reflexions with Miller indices $h-k=3n$) on a number of X-ray patterns.

We then superimposed the continuous line mentioned above on these Gaussian intensity distribu-

Table 9. $[\gamma]'_3$ *and* $[\gamma]'_4$ *values*

	Determined from the stackings of the 48-layer and 96-layer polytype models: 48-layer	96-layer	Calculated by the present method for the artificially faulted structures based on the 48-layer and 96-layer polytype models: 48-layer	96-layer
	$[\gamma]'_3$		$[\gamma]'_3$	
[000]′	0·042	0·042	0·057	0·044
[001]′	0·083	0·094	0·094	0·080
[010]′	0·083	0·083	0·108	0·116
[011]′	0·167	0·156	0·157	0·158
[100]′	0·083	0·094	0·094	0·080
[101]′	0·167	0·146	0·172	0·194
[110]′	0·167	0·156	0·157	0·158
[111]′	0·208	0·229	0·161	0·170
	$[\gamma]'_4$		$[\gamma]'_4$	
[0000]′	0·020	0·021	0·024	0·032
[0001]′	0·020	0·021	0·024	0·028
[0010]′	0·042	0·042	0·028	0·045
[0011]′	0·042	0·052	0·075	0·066
[0100]′	0·042	0·042	0·028	0·045
[0101]′	0·042	0·042	0·075	0·075
[0110]′	0·042	0·031	0·034	0·028
[0111]′	0·125	0·125	0·128	0·112
[1000]′	0·020	0·021	0·024	0·028
[1001]′	0·063	0·072	0·079	0·083
[1010]′	0·042	0·042	0·075	0·075
[1011]′	0·125	0·104	0·087	0·073
[1100]′	0·042	0·052	0·075	0·066
[1101]′	0·125	0·104	0·087	0·073
[1110]′	0·125	0·125	0·128	0·112
[1111]′	0·083	0·104	0·029	0·059

tions, and using the adequate values of the resulting intensity curves $\pi'(m,p)$ sets were calculated using the procedure given in part I. Some sets of these values based on a 48 and a 96-layer polytype are given in Table 8.

It can be seen in the first two sets of $\pi'(m,p)$ values [Table 8(*c*)] that by introducing even one single stacking fault between two identical 48-layer regions when building up the 96-layer polytype model, the values in the π' sets observably changed. Thus we could expect a more considerable change in the π' values calculated from the intensity distribution of the artificially made faulted structures than obtained in the case described above; nevertheless they are supposed to approach the values of the $\pi'(m,p)$ sets of pure model polytypes.

As Table 8 proves there is really a considerable difference between corresponding values of $\pi'(m,p)$ in Table 8(*c*) and (*d*), but the mean value of the difference does not exceed 16%.

Consequently, since the determination of $[\gamma]'_3$ and $[\gamma]'_4$ values is based on the adequate $\pi'(m,p)$ sets, we can expect that if our method for their determination is correct, the $[\gamma]'_p$ values thus determined by it for the faulted structure will not greatly differ from the $[\gamma]'_p$ values of their parent polytype models. The latter can be determined simply by counting the identical structure elements in the stacking of the model polytypes.

Strictly speaking, while all formulae for the determination of $[\gamma]'_3$ and $[\gamma]'_4$ values are linear relations of $\pi'(m,p)$'s, the difference between related $[\gamma]'_p$ pairs may not exceed the mean value of the difference in $\pi'(m,p)$ values multiplied by the number of π's in the corresponding formula. Since the mean value of the difference is not greater then 30% [about twice the mean difference of the $\pi'(m,p)$ values] derived from the data of Table 9, where $[\gamma]'_3$ and $[\gamma]'_4$ sets calculated from the $\pi'(m,p)$ sets of the faulted models are given, together with the $[\gamma]'_p$ values of the pure polytypes, the error induced by the assumptions is within the limits of the experimental error.

Conclusion

Starting from the direct method for determining the stacking sequence of polytypes with periodic structure a new procedure has been worked out to obtain values characteristic of lattices with stacking faults. These characteristic values are the relative rates of occurrence of structure elements ($[\gamma]'_2$, $[\gamma]'_3$ and $[\gamma]'_4$) consisting of three, four and five subsequent layers of the lattice.

As starting values a $\pi'(m,p)$ set calculated from the measured intensities on the X-ray pattern is needed. Formulae for the determination of $[\gamma]'_2$ and $[\gamma]'_3$ are given in part I (Farkas-Jahnke, 1973). In this paper the method for the determination of $[\gamma]'_4$ values has been outlined.

The procedure may be summarized by the following. There are two types of starting values:

(*a*) The set of $\pi'(m,p)$ values is symmetrical in m $[\pi'(m,p)=\pi'(-m,p)]$

or

(*b*) the set of $\pi'(m,p)$ values is asymmetrical.

For (a)

(1) Assuming that $[\gamma]'_4$ values are also symmetrical, we calculate the limits for their possible values according to the formulae in Table 4. (If any of the limiting values turn out to be less than zero, corrections have to be made until all values become greater than or equal to 0.)

(2) By calculating the mean value of $[\gamma]'_{4\,\max}$ and $[\gamma]'_{4\,\min}$ we have a set of $[\gamma]'_{4s}$ values ($[\gamma]'_{4s\,\text{mean}}$).

For (b)

(1) From the set of asymmetrical $\pi'(m,p)$'s a symmetrical $\pi'(m,p)$ set has to be calculated according to equation (8).

(2) By the procedure described for case (*a*) a set of $[\gamma]'_{4s}$ values is obtained.

(3) From these $[\gamma]'_{4s}$ values the asymmetrical $[\gamma]'_4$ values belonging to the first group (*i.e.* $[0]'_4$, $[1]'_4$, $[6]'_4$, $[7]'_4$, $[8]'_4$, $[9]'_4$, $[14]'_4$, $[15]'_4$) are calculated by the formulae given in Table 5.

(4) For $[\gamma]'_4$'s belonging to the second group limits can only be determined by using the $[\gamma]'_{4s}$ values. After having determined these limits by using the equations in Table 6, the mean values of $[\gamma]'_{4\,\max}$ and $[\gamma]'_{4\,\min}$ give the missing group of the $[\gamma]'_4$ values, *i.e.* $[2]'_4$, $[3]'_4$, $[4]'_4$, $[5]'_4$, $[10]'_4$, $[11]'_4$, $[12'_4$, $[13]'_4$.

Supplement to case (a)

(3) If the $\pi'(m,p)$ set is symmetrical, the first group of $[\gamma]'_4$'s, dependent only on $[1]'_4$ is symmetrical also.

(4) The group of $[\gamma]'_4$ depending also on $[2]'_4$ (the second group of $[\gamma]'_4$ values) is not necessarily symmetrical, only if $[2]'_4=[4]'_4$. The conditions for this case are given in Table 8.

By having determined all $[\gamma]'_4$ values, we obtain in fact fault parameters of the lattice, taking into account interactions between five successive layers.

References

DORNBERGER-SCHIFF, K. & FARKAS-JAHNKE, M. (1970). *Acta Cryst.* A**26**, 24–34.

DORNBERGER-SCHIFF, K. (1972). *Kristallografiya*, **16**, 1247–1252.

FARKAS-JAHNKE, M. (1971). First European Conference on the Physics of Condensed Matter, Abstract No. 65.

FARKAS-JAHNKE, M. (1973). *Acta Cryst.* B**29**, 407–413.