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The Diffraction of X-rays by Close-Packed Polytypic Crystals Containing Single Stacking Faults. II. Theory for Hexagonal and Rhombohedral Structures

By E. Michalski, S. Kaczmarek and M. Demianiuk

Institute of Technical Physics, Military Academy of Technology, 00 908 *Warsaw, Poland*

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Abstract

The general theory developed by Michalski [*Acta Cryst.* (1988), A**44**, 640–649] has been applied to the cases of hexagonal and rhombohedral structures. The symbols of stacking faults based on Zhdanov's symbols of local structure near the faults have been introduced and assigned to the formal subscripts *j*, *k* used in general theory. On this basis the regularities, according to which the faults with different subscripts *j*, *k* have the same structures, have been characterized. Then these regularities have been taken into consideration in the derivation of expressions for measurable parameters of changes (caused by faults) in the X-ray intensity distribution. The results obtained for structures $2H$, $4H$, $6H(33)$, $8H(44)$, $10H(55)$, $12H(66)$, $3C$, $9R(12)_3$, $12R(13)_3$ and $15R(23)_3$ are given. Some results are compared with published data. The physical meaning of the assumption of small values of fault probabilities is discussed.

1. Introduction

Warren (1959) has indicated that two types of stacking faults can occur in the simplest case of hexagonal polytypes with $2H$ structure. The probability of occurrence of the so-called deformation fault with the layer sequence ... $ABAB:CACA$ ... is denoted by α and of the growth fault with the layer sequence ... $ABAB:CBCB$ ... by β. Warren (1959) showed that there are no X-ray diffraction peak displacements and no peak asymmetry as a result of either deformation or growth faults, but peak broadening does occur.

In the case of hexagonal polytypes with $4H$ structure Prasad & Lele (1971) distinguished the following types of possible faults: intrinsic *c*, *h*, 2*c*, 2*h*, 3*c*, 3*h*, *ch* and extrinsic 4*c* and *cch*. The probabilities of occurrence of these faults have been denoted by the above symbols written as subscripts to α. The integrated intensity, peak shifts, peak broadenings and peak asymmetry have been chosen as measurable parameters of changes in the X-ray intensity distribution caused by the faults. The seven independent combinations of fault probabilities evaluated by Prasad & Lele (1971) show the influence of all possible faults on the above parameters.

For the case of $6H(33)$ polytypic structures Pandey & Krishna (1976) denoted the probabilities of occurrence of the intrinsic faults by symbols α_i. In this notation the subscripts *i* are the successive numbers, from 1 to 18, assigned to particular faults. Pandey & Krishna (1976) summarized the diffraction effects in the faulted $6H(33)$ structure as follows: (i) reflexions with $H-K\neq 3N$ are unaffected by faulting; (ii) all reflexions with $H-K=3N$ are broadened as a result of faulting; (iii) there is change in the intensity of the peak maxima; and (iv) reflexions with $H-K\neq 3N$, $L=6M\pm 1$ and $L=6M\pm 2$ also exhibit peak shifts.

A description of the influence of the faults on the X-ray diffraction pattern for the case of the $8H(44)$ polytypic structure has been given by Michalski, Demianiuk, Kaczmarek & Zhmija (1981).

For hexagonal polytypes, with the period of identity more than 8, there is no earlier description of the influence of the faults on X-ray diffraction patterns.

In the simplest case of rhombohedral structure, *i.e.* that of the $3C$ structure, the symbols α and β were sufficient for fault notation. Following Warren (1959) the probability of occurrence of single deformation faults is denoted by α and twin or growth faults by β. The deformation faults give rise to the shifts, broadenings and asymmetry of reciprocal-lattice points, whereas the twin faults produce only the broadenings (Warren, 1959).

In the case of the $9R(12)_3$ structure, symbols *c*, *h*, *hc*, *hhc* and 3*c* have been used by Lele (1974*a*) for notation of different stacking faults. From the process of fault formation, the first three have been called growth faults and the next two deformation faults. From the description of X-ray diffraction given by Lele (1974*a*) all the faults exert some influence on the width of reflexions. The integrated intensity and peak asymmetry are influenced by *h*, *hc*, *hhc* and 3*c* faults, whereas peak shifts are due to *c*, *hhc* and 3*c* faults.

In the case of $12R(13)_3$ structures Lele (1974*b*) used the symbols *hhc*, *c*, *h*, *cch*, 4*h*, 2*hc* and 4*c* for notation of different stacking faults. The differenti-

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ation of faults is introduced as for $9R(12)_3$ structures. The first four symbols refer to growth faults and the next three to deformation faults. All the faults influence the width of reflexions. The integrated intensity and peak asymmetry are influenced by *h*, *cch*, 4*h*, 2*ch* and 4*c* faults.

It can be seen that only some types of faults in $9R(12)_3$ and $12R(13)_3$ structures have been considered by Lele (1974*a*, *b*). For rhombohedral polytypes with a longer period of identity the description of X-ray diffraction has not yet been published.

2. Structures of stacking faults in hexagonal and rhombohedral polytypes

For synonymous and uniform notation of the faultiness of structures, we shall use Zhdanov symbols of crystal structure near the faults. This notation contains in brackets the numbers of the Zhdanov symbol, which are different from the numbers occurring on the same positions in the symbol for a perfect structure. Moreover, the last number of the Zhdanov symbol, which is not changed as a result of faults, exists before the bracket. The notation for twinning faults also contains the first number of the Zhdanov symbol which is after the bracket. In the $nH(\frac{n}{2}\frac{n}{2})$ type of structure the Zhdanov symbols contain only one repeated number. In these cases, for notation of faults, it is sufficient to give only the numbers occurring in brackets.

In order to illustrate the method of formation of the Zhdanov symbols for faults let us consider in detail two cases of faults, in $6H(33)$ and in $9R(12)_3$ structures.

The perfect sequences of layers in the $6H(33)$ structure are given below:

$$A_1B_2C_3A_4C_5B_6,$$
$$B_1C_2A_3B_4A_5C_6,$$
$$C_1A_2B_3C_4B_5A_6.$$

If the faulted layers (forming the faults) with subscripts 1 (*e.g.* C_1) occur after a layer with subscript 1 (*e.g.* A_1) instead of the perfect layer with subscript 2 (*e.g.* B_2), then we obtain the following sequence near the fault:

$$\ldots A_1^+B_2^+C_3^+A_4^-C_5^-B_6^-A_1^-:C_1^+A_2^+B_3^+C_4^-B_5^-A_6^- \ldots \quad (1)$$

On the basis of (1) we can see that the number of '−' signs in the Hägg symbol for this sequence increases by one. Hence the number (4) occurs in the Zhdanov symbol of this fault.

Table 1. *Zhdanov symbols for single non-twinning faults for particular values of subscripts j, k*

(*a*) Structure 4*H*

k \ *j*	1	2	3	4
1	(3)	(11)	(5)	(13)
2	(31)	(111)	(4)	(1)
3	(5)	(13)	(3)	(11)
4	(4)	(1)	(31)	(111)

(*b*) Structure $9R(12)_3$

k \ *j*	1	2	3	4	5	6	7	8	9
1	1 (3)	2 (3)	1 (12)	1 (3)	2 (3)	1 (12)	1 (3)	2 (3)	1 (12)
2	1 (5)	2 (2)	1 (1)	1 (5)	2 (2)	1 (1)	1 (5)	2 (2)	1 (1)
3	1 (4)	2 (21)	1 (111)	1 (4)	2 (21)	1 (111)	1 (4)	2 (21)	1 (111)
4	1 (3)	2 (3)	1 (12)	1 (3)	2 (3)	1 (12)	1 (3)	2 (3)	1 (12)
5	1 (5)	2 (2)	1 (1)	1 (5)	2 (2)	1 (1)	1 (5)	2 (2)	1 (1)
6	1 (4)	2 (21)	1 (111)	1 (4)	2 (21)	1 (111)	1 (4)	2 (21)	1 (111)
7	1 (3)	2 (3)	1 (12)	1 (3)	2 (3)	1 (12)	1 (3)	2 (3)	1 (12)
8	1 (5)	2 (2)	1 (1)	1 (5)	2 (2)	1 (1)	1 (5)	2 (2)	1 (1)
9	1 (4)	2 (21)	1 (111)	1 (4)	2 (21)	1 (111)	1 (4)	2 (21)	1 (111)

The perfect sequences of layers in $9R(12)_3$ structures are

$$A_1B_2A_3C_4A_5C_6B_7C_8B_9,$$
$$B_1C_2B_3A_4B_5A_6C_7A_8C_9,$$
$$C_1A_2C_3B_4C_5B_6A_7B_8A_9.$$

If a faulted layer with subscript 2 (*e.g.* C_2) occurs after a layer with subscript 2 (*e.g.* B_2) instead of a perfect layer with subscript 3 (*e.g.* A_3) then we obtain the following sequence near the fault:

$$\ldots C_6^-B_7^+C_8^-B_9^-A_1^+B_2^+:C_2^-B_3^-A_4^+B_5^-A_6^- \ldots \quad (2)$$

From (2) it is clear that the structure near the fault can be described by the Zhdanov symbol 2(2).

For a hexagonal structure, due to 6_3 screw axes, the Zhdanov symbol consists of an odd set of numbers repeated twice. Hence the set of $n^2/2$ types of faults are also repeated twice. Specific regularities exist in these repetitions. In order to illustrate these regularities, the Zhdanov symbols corresponding to all subscripts *j*, *k* for 4*H* structures are given in Table 1(*a*). From this table we can find that the Zhdanov symbols of faults are the same for pairs of subscripts (j, k) and $(j+n/2, k+n/2)$. Thus for hexagonal polytypes it is sufficient to give the Zhdanov symbols of $n^2/2$ faults.

The Zhdanov symbols corresponding to all the pairs of subscripts *j*, *k* for the non-twinning faults in $9R(12)_3$ rhombohedral structures are given in Table 1(*b*). The group of faults denoted by subscripts *j*, $k = 1, 2, \ldots, n/3$ are repeated nine times in this table. This property is characteristic of all rhombohedral polytypes because the Zhdanov symbols for them consist of sets of numbers repeated three times.

It can be shown that pairs of faults, which are enantiomorphous with others, exist among the $n^2/2$ types of faults in hexagonal structures and $n^2/9$ types of faults in rhombohedral structures. Such enantiomorphous pairs of faults give identical X-ray diffraction patterns by the rotation crystal method. Therefore we have to consider these faults as the same fault twice repeated, as was done by Pandey & Krishna (1976) for the $6H(33)$ structure. Thus the number of really different types of faults is less than $n^2/2$ in hexagonal structures and $n^2/9$ in rhombohedral structures. As an example let us consider the faults in $nH(\frac{n}{2}\frac{n}{2})$-type structures. The faults denoted by the Zhdanov symbols $(n+1)$, $(n), \ldots, (\frac{n}{2}+1)$ which occur after layers with subscripts $j=1$ and the faults denoted by the Zhdanov symbols $(j-1)$, $(j-1, j-1)$ and $(j-1, 1, j-1)$ which occur after layers with subscripts $j=2, 3, \ldots, \frac{n}{2}$ are non-repeated. The full number of these faults is

$$[(n/2+1)+3(n/2-1)]=2n-2. \qquad (3)$$

From among the remaining $[n(n/2)-(2n-2)]$ types of faults only half are different in reality. Thus the number of all possible different types of faults in $nH(\frac{n}{2}\frac{n}{2})$ structures is

$$\tfrac{1}{2}[n(n/2)-(2n-2)]+(2n-2)=(n^2/4)+n-1. \qquad (4)$$

For individual polytypic structures we obtain the following numbers of the possible types of faults: seven for $4H$, 14 for $6H(33)$, 23 for $8H(44)$, 34 for $10H(55)$, 47 for $12H(66)$ *etc.*

Similarly, in the $9R(12)_3$ structure, there exist the following pairs of enantiomorphous faults: 2(21)-1(12), 1(4)2-2(4)1, 1(3)2-2(3)1 and 1(31)1-1(13)1.

3. The parameters of changes in the intensity distribution

From the previous section it is known that in hexagonal structures the faults denoted by pairs of subscripts

$$(j, k) \quad \text{and} \quad (j+n/2, k+n/2) \qquad (5)$$

and in the rhombohedral structures faults denoted by

$$\begin{gathered}(j, k), \quad (j+n/3, k), \quad (j+2n/3, k), \\ (j, k+n/3), \quad (j+n/3, k+n/3), \\ (j+2n/3, k+n/3), \quad (j, k+2n/3), \\ (j+n/3, k+2n/3), \quad (j+2n/3, k+2n/3)\end{gathered} \qquad (6)$$

have the same sequences of layers. Since these faults are indistinguishable, we ought to consider them as one type of fault repeated twice in hexagonal structures and repeated nine times in rhombohedral structures. Let us denote the probability of occurrence of this type of fault by $\alpha_{\langle jk\rangle}$.

In order to express the measurable parameters of changes in the intensity distribution by probabilities $\alpha_{\langle jk\rangle}$, we shall apply the general theory developed in paper I (Michalski, 1988).

From the symmetry of the Hägg symbols one can write the following relationship between the factors S_j:

for hexagonal structures,

$$S_{j+n/2}=S_j^*; \qquad (7)$$

for rhombohedral structures,

$$S_j=S_{j+n/3}=S_{j+2n/3}. \qquad (8)$$

Combining (7) and (8) with the definition of the factors S_{jk} [equation (44) of paper I] we obtain:

for hexagonal sttructures,

$$S_{j+n/2,\,k+n/2}=S_{jk}^*, \qquad (9)$$

where S_{jk}^* means the complex conjugate of S_{jk};

for rhombohedral structures,

in the case of non-twinning faults

$$\begin{aligned}&S_{jk}=S_{j+n/3,\,k+n/3}=S_{j+2n/3,\,k+2n/3},\\ &S_{j+n/3,\,k}=S_{j+2n/3,\,k+n/3}=S_{j,\,k+2n/3}=S_{jk}\prod_{i=1}^{n/3}S_i, \qquad (10)\\ &S_{j+2n/3,\,k}=S_{j,\,k+n/3}=S_{j+n/3,\,k+2n/3}=S_{jk}\prod_{i=1}^{n/3}S_i^*;\end{aligned}$$

in the case of twinning faults

$$\begin{aligned}&S_{jk}=S_{j,\,k+n/3}=S_{j,\,k+2n/3},\\ &S_{j+n/3,\,k}=S_{j+n/3,\,k+n/3}=S_{j+n/3,\,k+2n/3}=S_{jk}\prod_{i=1}^{n/3}S_i, \qquad (11)\\ &S_{j+2n/3,\,k}=S_{j+2n/3,\,k+n/3}=S_{j+2n/3,\,k+2n/3}=S_{jk}\prod_{i=1}^{n/3}S_i^*.\end{aligned}$$

Substituting (9) into the general theory we obtain the following characteristic equations for hexagonal structures:

when $k\le j$,

$$X^n-\alpha_{\langle jk\rangle}(S_{jk}+S_{jk}^*)X^{n+k-j-1}+2\alpha_{\langle jk\rangle}-1=0; \qquad (12)$$

when $k>j$,

$$X^n-\alpha_{\langle jk\rangle}(S_{jk}+S_{jk}^*)X^{k-j-1}+2\alpha_{\langle jk\rangle}-1=0. \qquad (13)$$

Because $\mathrm{Re}(S_{jk}+S_{jk}^*)=2\,\mathrm{Re}\,S_{jk}$, (12) and (13) differ from equations (22) and (23) of the general theory only in the occurrence of the symbols $2\alpha_{\langle jk\rangle}$ instead of α_{jk}. We can prove that the terms $J^0(m)$ of the boundary conditions for hexagonal structures are real. Thus the final formulae for Δh_3, Δw and I_{max} in hexagonal structures can be obtained by substituting the $2\alpha_{\langle jk\rangle}$ instead of α_{jk} in the general formulae [equations (43), (48), (50) and (52) of paper I].

Similarly using (10) and (11) we obtain the following characteristic equations for rhombohedral structures:

in the case of non-twinning faults,

$$X^n - 3\alpha_{\langle jk\rangle}S_{jk}X^{n+k-j-1}\left(1+\prod_{i=1}^{n/3} S_iX^{-n/3}+\prod_{i=1}^{n/3} S_iX^{n/3}\right) + 9\alpha_{\langle jk\rangle} - 1 = 0, \quad \text{for} \quad k \le j, \tag{14}$$

$$X^n - 3\alpha_{\langle jk\rangle}S_{jk}X^{k-j-1}\left(1+\prod_{i=1}^{n/3} S_iX^{-n/3}+\prod_{i=1}^{n/3} S_iX^{n/3}\right) + 9\alpha_{\langle jk\rangle} - 1 = 0, \quad \text{for} \quad k > j; \tag{15}$$

in the case of twinning faults,

$$X^n + 9\alpha_{\langle jk\rangle} - 1 = 0. \tag{16}$$

From the characteristic equations (14), (15) and (16) we can find the coefficients a_j and D_m. After substituting them in the general equations for Δh_3 and Δw [equations (42) and (47) of paper I] and some rearrangements we obtain finally:

in the case of non-twinning faults,

$$\Delta h_3(h_3, \alpha_{\langle jk\rangle}) = \alpha_{\langle jk\rangle}(9/4\pi)\sin[2l(\pi/n)h_3] \tag{17}$$

and

$$\Delta w(h_3, \alpha_{\langle jk\rangle}) = \alpha_{\langle jk\rangle}(9/2\pi)\{5-4\cos[2l(\pi/n)h_3] - \sin^2[2l(\pi/n)h_3]\}^{1/2}, \tag{18}$$

where

$$l = \begin{cases} k-j-1 & \text{for} \quad S_{jk}=1, \\ k-j-1-n/3 & \text{for} \quad S_{jk}=\prod_{i=1}^{n/3} S_i^*, \\ k-j-1+n/3 & \text{for} \quad S_{jk}=\prod_{i=1}^{n/3} S_i; \end{cases} \tag{19}$$

in the case of twinning faults

$$\begin{aligned} \Delta h_3(h_3, \alpha_{\langle jk\rangle}) &= 0, \\ \Delta w(h_3, \alpha_{\langle jk\rangle}) &= \alpha_{\langle jk\rangle}(9/\pi). \end{aligned} \tag{20}$$

From (17) to (20) shifts and broadenings of reciprocal-lattice points may be caused by non-twinning faults whereas the twinning faults do not cause shifts. Broadenings for all indexes h_3 are caused by all types of twinning faults.

The influence of stacking faults on the intensity peak maxima in rhombohedral polytypes is expressed by equation (52) of paper I, because the terms $J^0(m)$ in the boundary conditions are complex.

Moreover, it can be shown that for enantiomorphous pairs of faults terms $2\alpha_{\langle jk\rangle}$ instead of $\alpha_{\langle jk\rangle}$ ought to be substituted in the final expressions for Δh_3, Δw and I_{max}.

4. Results of calculations for 2*H*, 4*H*, 6*H*(33), 8*H*(44), 10*H*(55), 12*H*(66), 3*C*, 9*R*(12)$_3$, 12*R*(13)$_3$ and 15*R*(23)$_3$ structures

In order to present the result in the shortest and most convenient form, we list them in Table 2. This table allows the shifts Δh_3, broadenings Δw and changes in the maximum intensity of the reciprocal-lattice points to be expressed by the probabilities of occurrence of all possible faults. To express Δh_3, for example, by probabilities of particular faults we need to multiply the values from the table corresponding to the particular α and h_3 by the reciprocal coefficients which occur before Δh_3 in the heading of the table. In the case of faults united by the '=' sign we multiply Δh_3 and Δw and divide $I_{max}(h_3)$ additionally by a factor 2. The values of l assigned to rhombohedral structures for all fault types are determined by (19). The absence of numbers in the table for some peak maxima means that the peak maximum of adequate reciprocal-lattice points is unaffected by this fault.

5. Discussion

The results obtained for shifts Δh_3 and broadenings Δw of reciprocal-lattice points in 2*H* structures (Table 2*a*) are in accordance with Warren's (1959) results.

The results obtained for the shifts Δh_3 and broadenings Δw of reciprocal-lattice points in 4*H* structures (Table 2*b*) are the same as those of Prasad & Lele (1971), although in order to describe faultiness these authors have used two more faults (*cch* and 4*c*) than here; but these [which have Zhdanov symbols (41) and (6)] are not single faults.

The full results obtained for 6*H*(33) structures (Table 2*c*) are identical to those given by Pandey & Krishna (1976).

For the 8*H*, 10*H* and 12*H* structures no comparison has been given because there are no corresponding results in earlier published papers.

According to Warren (1959), the following relation for 3*C* structures holds:

$$\Delta h_3\ (h_3 = \pm 1, \alpha) = \pm(3\sqrt{3}/4)\alpha, \tag{21}$$

Table 2. *Shifts Δh_3, broadenings Δw and peak maxima I_{max} of reciprocal-lattice points for particular α_{jk} probabilities*

(*a*) Structure $2H$

Zhdanov symbol of fault	$(1/\alpha_{(i)})\Delta h_3(h_3)$, h_3: ±1, ±2	$(\pi/\alpha_{(i)})\Delta w(h_3)$, h_3: ±1	±2	$(3\alpha_{(i)}/\psi^2)I_{max}(h_3)$, h_3: ±1	±2
(2)	0	1	3	9	1
(3)	0	3	3	3	1

(*b*) Structure $4H$

Zhdanov symbol of fault	$(2\pi/\alpha_{(i)})\Delta h_3(h_3)$, h_3: $4M\pm1$	$(\pi/\alpha_{(i)})\Delta w(h_3)$, h_3: $4M$	±1	±2	$(\alpha_{(i)}/\psi^2)I_{max}(h_3)$, h_3: $4M$	±1	±2
(4)	0	3	1	3	1/6	3/2	3/2
(5)	±2	0	2	4	—	3/4	9/8
(1)	±1	3	2	1	1/6	3/4	9/2
(31) = (13)	0	3	3	3	1/6	1/2	3/2
(3), (111)	±1	3	2	1	1/6	3/4	9/2
(11)	0	0	4	0	—	3/8	—

(*c*) Structure $6H(33)$

Zhdanov symbol of fault	$(4\pi/3\alpha_{(i)})\Delta h_3(h_3)$, h_3: $6M\pm1$	$6M\pm2$	$(2\pi/\alpha_{(i)})\Delta w(h_3)$, h_3: ±1	±2	±3	$(\alpha_{(i)}/\psi^2)I_{max}(h_3)$, h_3: ±1	±2	±3
(5)	±1	∓1	3	3	6	2/3	2	4/3
(6)	0	0	8	0	8	1/4	—	1
(12) = (21)	0	0	2	6	2	1/2	1/2	2
(7), (1)	∓1	±1	3	3	6	2/3	2	4/3
(22)	±2	∓2	6	6	0	1/3	1	—
(14) = (41)	±2	±2	2	6	8	1/2	1/2	1/2
(2)	∓1	∓1	5	3	2	2/5	2	4
(111), (42) = (24)	0	0	6	6	6	1/3	1	4/3
(4), (211) = (112)	±1	±1	5	3	2	2/5	2	4
(11), (212)	∓2	±2	6	6	0	1/3	1	—

(*d*) Structure $8H(44)$: shifts $(4\pi/\alpha_{(i)})\Delta h_3(h_3)$

Number	Zhdanov symbol of faults	h_3: $8M\pm1$	$8M\pm2$	$8M\pm3$
1	(6)	±2	0	∓2
2	(7)	∓2√2	±4	∓2√2
3	(313), (12) = (21)	±√2	∓2	±√2
4	(13) = (31), (8)	0	0	0
5	(53) = (35), (112) = (211)	0	0	0
6	(22)	0	0	0
7	(1)	±2√2	∓4	±2√2
8	(9), (23) = (32)	∓√2	±2	∓√2
9	(33)	±4	0	∓4
10	(2), (51) = (15)	∓2	0	±2
11	(111), (52) = (25)	±2√2	±4	±2√2
12	(3)	±√2	∓2	∓√2
13	(5), (113) = (311), (212)	±√2	±2	±√2
14	(11), (213) = (312)	∓4	0	±4

(*e*) Structure $8H(44)$: broadenings $(\pi/\alpha_{(i)})\Delta w(h_3)$

Number	h_3: $8M$	$8M\pm1$	$8M\pm2$	$8M\pm3$	$8M\pm4$
1, 10	3	2	1	2	3
2, 7	0	√2+2	2	√2−2	4
3, 8	3	1/2(√2−4)	2	1/2(√2+4)	1
4	3	1	3	1	3
5	3	3	3	3	3
6	0	4	0	4	0
9, 14	0	2	4	2	0
11	0	√2−2	2	√2+2	4
12, 13	3	1/2(√2+4)	2	1/2(√2−4)	1

(*f*) Structure $8H(44)$: peak maxima $(\alpha_{(i)}/\psi^2)I_{max}(h_3)$

Number	h_3: $8M$	$8M\pm1$	$8M\pm2$	$8M\pm3$	$8M\pm4$
1, 10	1/12	3/8(3−2√2)	9/4	3/8(3+2√2)	1/4
2, 7	—	3/8(10−7√2)	9/8	3/8(10+7√2)	9/16
3, 8	1/12	3/28(8−5√2)	9/8	3/28(8+5√2)	9/4
4	1/12	3/4(3−2√2)	1/4	3/4(3+2√2)	1/4
5	1/24	1/8(3−2√2)	3/8	1/8(3+2√2)	3/8
6	—	3/16(3−2√2)	—	3/16(3+2√2)	—
9, 14	—	3/8(3−2√2)	9/16	3/8(3+2√2)	—
11	—	3/8(2−√2)	9/8	3/8(2+√2)	9/16
12, 13	1/12	3/28(16−√2)	9/8	3/28(16+√2)	9/4

(*g*) Structure $10H(55)$: shifts $(2\pi/\alpha_{(i)})\Delta h_3(h_3)$

Number	Zhdanov symbol of faults	h_3: $10M\pm1$	$10M\pm2$	$10M\pm3$	$10M\pm4$
1	(7)	±b	±a	∓a	∓b
2	(8)	∓2b	±2a	±2a	∓2b
3	(12) = (21)	±b	∓a	∓a	±b
4	(22)	∓2a	±2b	∓2b	±2a
5	(13) = (31), (9), (414)	±a	∓b	±b	∓a
6	(1), (24) = (42)	∓a	±b	∓b	±a
7	(2)	±2b	∓2a	∓2a	±2a
8	(16) = (61), (34) = (43)	∓b	±a	±a	∓b
9	(44)	±2b	±2a	∓2a	∓2b
10	(26) = (62), (111), (3)	∓b	∓a	±a	±b
11	(36) = (63), (112) = (211)	±2a	±2b	±2b	±2a
12	(4)	∓a	∓b	∓b	∓a
13	(6), (114) = (411), (213) = (312)	±a	±b	±b	±a
14	(1, 1), (214) = (412), (313)	∓2b	∓2a	±2a	±2b
15	(314) = (413)	±b	∓a	∓a	±b
16	(14) = (41)	0	0	0	0
17	(11), (33)	0	0	0	0
18	(10), (23) = (32)	0	0	0	0
19	(113) = (311), (212), (46) = (64)	0	0	0	0

$a = \sin(\pi/5)$, $b = \sin(2\pi/5)$, $c = \cos(\pi/5)$, $d = \cos(2\pi/5)$.

(*h*) Structure $10H(55)$: broadenings $(\pi/\alpha_{(i)})\Delta w(h_3)$

Number	h_3: $10M$	$10M\pm1$	$10M\pm2$	$10M\pm3$	$10M\pm4$	$10M\pm5$
1, 10	3	g	f	f	g	3
2, 7	0	k	i	j	l	8
3, 8, 15	3	h	f	e	g	1
4, 17	0	i	l	l	i	0
5, 6	3	f	g	g	f	3
9, 14	0	l	i	i	l	0
11	0	j	l	k	i	4
12, 13	3	e	g	h	f	1
16	0	4	0	4	0	4
18	3	1	3	1	3	1
19	3	3	3	3	3	3

$e = \sqrt{(5+4c-a^2)} = 20{\cdot}8090$, $f = \sqrt{(5-4c-a^2)} = 1{\cdot}1910$, $g = \sqrt{(5+4d-b^2)} = 2{\cdot}3090$, $h = \sqrt{(5-4d-b^2)} = 1{\cdot}6910$, $i = 2\sqrt{(2+2c-a^2)} = 3{\cdot}6180$, $j = 2\sqrt{(2-2c-a^2)} = 0{\cdot}3820$, $k = 2\sqrt{(2+2d-b^2)} = 2{\cdot}6180$, $l = 2\sqrt{(2-2d-b^2)} = 1{\cdot}3820$.

(*i*) Structure $10H(55)$: peak maxima $(\alpha_{(i)}/\psi^2)I_{max}(h_3)$

Number	h_3: $10M$	$10M\pm1$	$10M\pm2$	$10M\pm3$	$10M\pm4$	$10M\pm5$
1, 10	0·067	0·02757	0·5773	3·4530	2·0410	0·2
2, 7	—	0·03343	0·1900	10·767	3·4100	0·0375
3, 8, 15	0·033	0·02588	0·2886	0·7320	1·1596	0·3
4, 17	—	0·02420	0·4975	2·9758	1·3025	—
5, 6	0·067	0·07350	0·0297	1·7810	3·9568	0·2
9, 14	—	0·06334	17·0498	1·1366	0·7121	—
11	—	0·11460	8·4562	0·7854	0·6512	0·075
12, 13	0·067	0·03116	0·2012	2·0925	3·9568	0·6
16	—	0·00486	—	0·2285	—	0·033
18	0·067	0·08754	0·2292	4·1125	1·5708	0·6
19	0·067	0·00973	0·2292	0·4569	1·5708	0·033

Table 2 (*cont.*)

(j) Structure $12H(66)$: shifts $(4\pi/\alpha_{(i)})\Delta h_3(h_3)$

Number	Zhdanov symbol of faults	h_3: $12M\pm1$	$12M\pm3$	$12M\pm4$	$12M\pm5$
1	(8)	±√3	0	∓√3	∓√3
2	(9)	∓4	±4	0	∓4
3	(12) = (21)	±2	∓2	0	±2
4	(22)	∓2√3	0	∓2√3	±2√3
5	(10), (13) = (31)	±√3	0	±√3	∓√3
6	(14) = (41)	∓2	∓4	±2√3	∓4
7	(11), (23) = (32)	±1	±2	∓√3	±1
8	(25) = (52)	±2	±2	∓2√3	∓2
9	(13), (1), (34) = (43)	∓1	∓2	±√3	∓1
10	(17) = (71), (44)	±2√3	0	±2√3	∓2√3
11	(35) = (53), (2)	∓√3	0	∓√3	±√3
12	(3)	±4	∓4	0	±4
13	(27) = (72), (45) = (54) (111)	∓2	±2	0	∓2
14	(55)	±2√3	0	∓2√3	∓2√3
15	(112) = (211), (4) (37) = (73)	∓√3	0	±√3	±√3
16	(113) = (311), (212) (47) = (74)	±2	±4	±2√3	±2
17	(5)	∓1	∓2	∓√3	∓1
18	(115) = (511), (313) (214) = (412), (7)	±1	±2	±√3	±1
19	(215) = (512), (1, 1) (314) = (413)	∓2√3	0	±2√3	±2√3
20	(315) = (513), (414)	±2	∓2	0	±2
21	(415) = (514)	±√3	0	±√3	±√3
22	(515)	∓2	∓4	±2√3	∓2
23	(12), (33)	0	0	0	0
24	(15) = (51), (24) = (42)	0	0	0	0
25	(114) = (411), (15) = (51) (213) = (312)	0	0	0	0

(k) Structure $12H(66)$: broadenings $(\pi/\alpha_{(i)})\Delta w(h_3)$

Number	h_3: $12M\pm1$	$12M\pm3$	$12M\pm4$	$12M\pm5$
1, 15	5/2	1	3/2	5/2
2, 12	2	2	0	2
3, 13, 20	2	2	3	2
4, 10	3	0	3	3
5, 11, 21	3/2	3	3/2	3/2
6, 8, 22	2+√3	2	3	2−√3
7, 9	1/2(4−√3)	2	3/2	1/2(4+√3)
14, 19	1	4	3	1
16	2−√3	2	3	2+√3
17, 18	1/2(4+√3)	2	3/2	1/2(4−√3)
23	4	4	0	4
24	1	1	3	1
25	3	3	3	3

(l) Structure $12H(66)$: peak maxima $(\alpha_{(i)}/\psi^2)I_{max}(h_3)$

Number	h_3: $12M\pm1$	$12M\pm3$	$12M\pm4$	$12M\pm5$
1, 15	2/5(2−√3)	2	4	2/5(2+√3)
2, 12	1/2(2−√3)	1/4	—	1/2(2+√3)
3, 13, 20	1/2(2−√3)	1	2	1/2(2+√3)
4, 10	1/3(2−√3)	—	2	1/3(2+√3)
5, 11, 21	2/3(2−√3)	2/3	4	2/3(2+√3)
6, 8, 22	7−4√3	1	2	7+4√3
7, 9	2/13(5−2√3)	1	4	2/13(5+2√3)
14, 19	2−√3	1/2	2	2+√3
16	1	5/2	2	1
17, 18	2/13(11−6√3)	1	4	2/13(11+6√3)
23	1/4(2−√3)	1/2	—	1/4(2+√3)
24	1/2(2−√3)	1	1	1/2(2+√3)
25	1/6(2−√3)	1/3	1	1/6(2+√3)

(m) Structure $3C$

	h_3: ±1	±2
Shifts $8/(9\sqrt{3}\alpha)\Delta h_3(h_3)$	±1	∓1
Broadenings $4\pi/(45\alpha)\Delta w(h_3)$	1	1
Peak maxima for non-twinning fault $(10^2\alpha^2)/(2{\cdot}74\psi^2)I_{max}(h_3)$	±1	∓1
Peak maxima for twinning fault $(10^2\beta^2)/(4{\cdot}28\psi^2)I_{max}(h_3)$	±1	∓1

(n) Structure $9R(12)_3$: shifts $(4\pi/9\alpha_{(i)})\Delta h_3(h_3)$

Zhdanov symbol of faults	l	h_3: $9M\pm1$	$9M\pm2$	$9M\pm4$
2 (3)	1	±b	±d	±a
1 (3)	2	±d	±a	∓b
1 (12) = 2 (21)	3	±c	∓c	±c
1 (4)	4	±a	∓b	∓d
1 (111), 2 (2)	5	±a	±b	±d
1 (5)	6	∓c	±c	∓c
1 (1)	7	∓d	∓a	±b

$a = \sin(\pi/9) = 0{\cdot}3420$, $b = \sin(2\pi/9) = 0{\cdot}6428$, $c = \sin(\pi/3) = 0{\cdot}8660$, $d = \sin(4\pi/9) = 0{\cdot}9848$.

(o) Structure $9R(12)_3$: broadenings $(\pi/\alpha_{(i)})\Delta w(h_3)$

l	h_3: $9M\pm1$	$9M\pm2$	$9M\pm4$
1	e	f	g
2, 7	f	g	e
3, 6	h	h	h
4, 5	g	e	f

$e = 5{\cdot}5528$, $f = 8{\cdot}2186$, $g = 13{\cdot}2286$, $h = 11{\cdot}25$.

(p) Structure $9R(12)_3$: peak maxima $[10^2\alpha_{(i)}^2/\psi^2(h_3)]I_{max}(h_3)$

l	h_3: $9M\pm1$	$9M\pm2$	$9M\pm4$
1	∓11·77	±2·29	∓7·33
2, 7	∓5·37	±0·88	∓41·60
3, 6	∓2·87	±1·22	∓10·13
4, 5	∓2·07	±5·02	∓18·98
Twinning faults	∓4·48	±1·91	∓15·83

(r) Structure $12R(13)_3$: shifts $(8\pi/9\alpha_{(i)})\Delta h_3(h_3)$

Zhdanov symbol of faults	l	h_3: $12M\pm1$	$12M\pm2$	$12M\pm4$	$12M\pm5$
3 (21) = 1 (12)	1	±1	±√3	±√3	±1
1 (5)	2	±√3	±√3	∓√3	∓√3
3 (2), 1 (112) = 1 (211)	3	±2	0	0	±2
1 (7)	4	±√3	∓√3	±√3	∓√3
1 (2)	5	±1	∓√3	∓√3	±1
1 (3)	6	0	0	0	0
1 (4)	7	±1	±√3	±√3	∓1
1 (111), 3 (22) = 1 (22)	8	∓√3	±√3	∓√3	±√3
1 (6)	9	∓2	0	0	∓2
1 (1), 1 (212)	10	∓√3	∓√3	±√3	±√3

(s) Structure $12R(13)_3$: broadenings $(4\pi/9\alpha_{(i)})\Delta w(h_3)$

l	h_3: $12M\pm1$	$12M\pm2$	$12M\pm4$	$12M\pm5$
1	4−√3	3	5	4+√3
2, 10	0	5	0	0
3, 9	4	6	2	4
4, 8	5	5	5	5
5, 7	4+√3	3	5	4−√3
6	6	2	2	6

(t) Structure $12R(13)_3$: peak maxima $[9\alpha_{(i)}^2/8\psi^2(h_3)]I_{max}(h_3)$

l	h_3: $12M\pm1$	$12M\pm2$	$12M\pm4$	$12M\pm5$
1	±(14−3√3)/169	∓1/9	±1/75	∓(14+3√3)/169
2, 10	—	∓1/25	±1/75	—
3, 9	±(2−√3)/16	∓1/36	±1/12	∓(2+√3)/16
4, 8	±(2−√3)/25	∓1/25	±1/75	∓(2+√3)/25
5, 7	±(7−5√3)²/338	∓1/9	±1/75	∓(7+5√3)²/338
6	±(2−√3)/36	∓1/4	±1/12	∓(2+√3)/36
Twinning faults	±(2−√3)/16	∓1/16	±1/48	∓(2+√3)/16

Table 2 (*cont.*)

(u) Structure $15R(23)_3$: shifts $(\pi/9\alpha_{(i)})\Delta h_3(h_3)$

Zhdanov symbol of faults	l	h_3: $15M\pm1$	$15M\pm2$	$15M\pm4$	$15M\pm5$	$15M\pm7$
3 (31) = 2 (13), 2 (7)	1	$\pm b$	$\pm d$	$\pm g$	$\pm e$	$\pm a$
3 (12) = 2 (21)	2	$\pm d$	$\pm g$	$\mp a$	$\mp e$	$\mp b$
3 (4)	3	$\pm f$	$\pm c$	$\mp f$	0	$\pm c$
2 (4), 3 (111)	4	$\pm g$	$\mp a$	$\pm b$	$\pm e$	$\mp d$
2 (23) = 3 (32), 2 (111)	5	$\pm e$	$\mp e$	$\pm e$	$\mp e$	$\pm e$
3 (13)	6	$\pm c$	$\mp f$	$\mp c$	0	$\mp f$
2 (1)	7	$\pm a$	$\mp b$	$\mp d$	$\pm e$	$\pm g$
2 (5)	8	$\mp a$	$\pm b$	$\pm d$	$\mp e$	$\mp g$
2 (112) = 2 (211), 3 (3)	9	$\mp c$	$\pm f$	$\pm c$	0	$\pm f$
2 (41) = 3 (14)	10	$\mp e$	$\pm e$	$\mp e$	$\pm e$	$\mp e$
2 (2)	11	$\mp g$	$\pm a$	$\mp b$	$\mp e$	$\pm d$
3 (5), 2 (6)	12	$\mp f$	$\mp c$	$\pm f$	0	$\mp c$
3 (11) = 2 (11), 2 (212)	13	$\mp d$	$\mp g$	$\pm a$	$\pm e$	$\pm b$

$a = \sin(\pi/15) = 0\cdot2079$, $b = \sin(2\pi/15) = 0\cdot4067$, $c = \sin(3\pi/15) = 0\cdot5878$, $d = \sin(4\pi/15) = 0\cdot7431$, $e = \sin(\pi/3) = 0\cdot8660$, $f = \sin(6\pi/15) = 0\cdot9511$, $g = \sin(7\pi/15) = 0\cdot9945$.

(v) Structure $15R(23)_3$: broadenings $(\pi/\alpha_{(i)})\Delta w(h_3)$

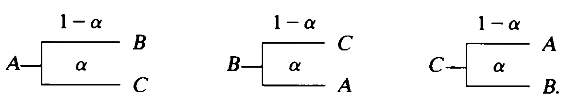
l	h_3: ±1	±2	±4	±5	±7
1	k	m	n	p	r
2, 13	m	n	r	p	k
3, 12	s	t	s	u	t
4, 11	n	r	k	p	m
5, 10	w	w	w	w	w
6, 9	t	s	t	u	s
7, 8	r	k	m	p	n

$k = 5\cdot53$, $m = 7\cdot63$, $n = 11\cdot39$, $p = 12\cdot53$, $r = 13\cdot47$, $s = 9\cdot72$, $t = 13\cdot18$, $u = 4\cdot50$, $w = 11\cdot25$.

(w) Structure $15R(23)_3$: peak maxima $[10^2\alpha_{(i)}{}^2/\psi^2(h_3)]I_{max}(h_3)$

l	h_3: $15M\pm1$	$15M\pm2$	$15M\pm4$	$15M\pm5$	$15M\pm7$
1	∓2·03	±4·09	∓7·19	±3·06	∓7·85
2, 13	∓1·07	±1·84	∓5·14	±3·06	∓46·54
3, 12	∓0·66	±1·37	∓9·87	±23·70	∓8·20
4, 11	∓0·48	±1·31	∓30·49	±3·06	∓24·46
5, 10	∓0·49	±1·88	∓7·37	±3·79	∓11·25
6, 9	∓0·36	±2·52	∓5·37	±23·70	∓15·07
7, 8	∓0·34	±7·78	∓16·20	±3·06	∓10·98
Twinning faults	∓6·06	±2·78	∓7·24	±8·89	∓17·91

where the probability α of the occurrence of deformation faults in the $3C$ structure is defined by the scheme

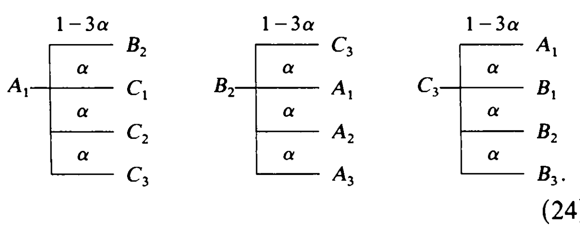


(22)

However in the present paper we have obtained the relation

$$\Delta h_3\ (h_3 = \pm1, \alpha_{\langle 11\rangle}) = \pm(9\sqrt{3}/8)\alpha_{\langle 11\rangle}, \quad (23)$$

where the probability $\alpha_{\langle 11\rangle}$ of occurrence of the single non-twinning faults with Zhdanov symbol (1) in the $3C$ structure is defined by the scheme



(24)

Comparing expressions (21) and (23) we obtain

$$\alpha_{\langle 11\rangle} = (2/3)\alpha. \quad (25)$$

The factor 2/3 occurs in (25) because the probabilities $\alpha_{\langle 11\rangle}$ and α are defined differently. To describe the faultiness in $3C$ structures the first scheme is more natural and convenient than the second one. By contrast, for rhombohedral polytypes with period of identity greater than 3 the $\alpha_{\langle jk\rangle}$ probabilities are more suitable.

The results obtained for $9R(12)_3$ and $12R(13)_3$ structures can be compared with results given by Lele (1974*a*, *b*). For the $9R(12)_3$ structure he obtained the following five types of faults: *c*, *h*, *hc*, *hhc* and 3*c*. The first three of these are non-twinning faults with Zhdanov symbols $c = 1(3)$, $hhc = 2(21)$ and $3c = 1(5)$. The next two are twinning faults with symbols $hc = 2(2)1$ and $h = 1(1)2$. For the $12R(13)_3$ Lele considered the following seven types of faults: *hhc*, *c*, *h*, *cch*, 4*h*, 2*hc* and 4*c*. The first five of these are non-twinning faults with symbols $hhc = 1(2)$, $c = 1(4)$, $4h = 1(111)$, $2hc = 1(22)$ and $4c = 1(7)$. The next two are twinning faults with symbols $h = 1(1)3$ and $cch = 3(3)1$.

Comparing the equations for shifts Δh_3 of the reciprocal-lattice points for $9R(12)_3$ and $12R(13)_3$ structures obtained from the tables with those given by Lele (1974*a*, *b*), we can see complete conformity. The shifts of reciprocal-lattice points are unaffected by twinning faults. For non-twinning faults the coefficients determining the magnitude of shifts and the direction of shifts given by Lele (1974*a*) conform with the data in our tables. The coefficients given by Lele (1974*a*, *b*) can be obtained in the following way:

$$0\cdot3949 = a/c, \quad 0\cdot7422 = b/c \quad \text{and} \quad 1\cdot1372 = d/c. \quad (26)$$

Comparing the expressions for broadening Δw of the reciprocal-lattice points calculated from the tables for $9R(12)_3$ and $12R(13)_3$ structures with expressions given by Lele (1974*a*, *b*), we can see some discrepancies.

Thus we can see that the general theory published in this paper gives the same results as obtained earlier for particular simple cases. However, the present theory allows easy calculations for all more complicated cases. The possibility of quick identification of the type of fault without exact measurements of X-ray diffraction patterns is the advantage of our tables. It is sufficient to determine the reflexions which are unaffected by faults and reflexions which are broadened and shifted in particular directions. Comparing such simple measurements with the tables we can identify the type of faults in the vast majority of cases, when the diffraction effects are distinct. Examples of this analysis will be given in a forthcoming paper. It seems, however, that the analysis of fault structures is not possible in the case of crystals which have total disorder (continuous diffuse lines instead of reflexions on X-ray diffraction photographs).

Moreover, we must pay attention to the fact that the different types of faults exert a similar influence on different points of the reciprocal lattice. Thus it is not possible to distinguish between some types of faults on the basis of the above parameters. One could try also to find expressions for measurable parameters describing lattice-point asymmetry and changes in the integrated intensity, as was done by Prasad & Lele (1971). However, these changes and peak asymmetry are usually too small to be estimated with sufficient accuracy. Thus peak shifts and half widths are recognized to be the best measures of faultiness. This was shown by Pandey & Krishna (1976) for the $6H(33)$ structure.

The limitations of our theory and inaccuracy in the results which follow from the assumption of small values of α_{jk} are the next problem for discussion. We will show that this assumption does not limit the generality of the above theory because only small values of α_{jk} have physical sense. In order to justify the above statement let us recall the definition of probability α_{jk}. It is equal to the ratio of the number of layers followed by faults of a particular type to the full number of layers in the examined sequence. For example, in the following sequence of an $8H(44)$ structure with stacking faults [(44334433444433444433344) - in Zhdanov symbols] we have $\alpha_{(33)}=4/80=0{\cdot}05$. It is clear that consideration of these faults as the (33) type in $8H(44)$ structures makes sense only for $\alpha_{(33)}<0{\cdot}1$. For $\alpha_{(33)}>0{\cdot}1$ the frequency of the occurrence of faults of (33) type is so great that the Zhdanov symbols (33) must be united in groups and it is necessary to interpret this sequence as a $6H(33)$ structure with stacking faults of (4) type. For example, it is necessary to interpret the sequence (33433433433334) as a $6H(33)$ structure with $\alpha_{(4)}=4/46$ but not as an $8H(44)$ structure with $\alpha_{(33)}=5/46$. We expect that on X-ray diffraction photographs from the structure with this sequence the peak maxima will occur near the positions corresponding to those for a $6H(33)$ structure.

The assumption of a random distribution of single faults does not limit our theory either. In general, when this assumption is not fulfilled another polytypic structure is formed.

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Direct Methods: the Identification of Conditions Which Simplify the Generation of Inconsistent Quadrupoles

BY DAVID A. LANGS AND FUSON HAN

Medical Foundation of Buffalo, Inc., 73 *High St, Buffalo, NY* 14203, *USA*

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Abstract

An algorithm is implemented to determine the form and phase shift for inconsistent type II quadrupoles for any space group having glide or screw-axis translations which are not a consequence of lattice centering. Cumulatively there are only six different Miller index restrictions and nine different phase shift forms common to all space groups of orthorhombic or lower symmetry. A similar analysis has been performed for a newly discovered type III class of quadrupoles. The configuration of the phase connections among the four triples of the type III quadrupole is different from the common configuration previously described for both normal (type I) and inconsistent (type II) quadrupoles. A knowledge of these constraint conditions for type II and III quadrupoles greatly simplifies a procedure for generating these relationships.

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Introduction

A quadrupole has been defined as a relationship among four interdependent three-phase invariants,

$$\begin{aligned}\Phi_1&=\varphi_{\mathbf{h}}-\varphi_{\mathbf{k}}+\varphi_{\mathbf{k-h}}\\ \Phi_2&=\varphi_{\mathbf{k}}-\varphi_{\mathbf{l}}+\varphi_{\mathbf{l-k}}\\ \Phi_3&=\varphi_{\mathbf{l}}-\varphi_{\mathbf{h}}+\varphi_{\mathbf{h-l}}\\ \Phi_4&=-\varphi_{\mathbf{k-h}}-\varphi_{\mathbf{l-k}}-\varphi_{\mathbf{h-l}},\end{aligned}\tag{1}$$