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The Influence of Crystal and Sample Symmetries on the Orientation Distribution Function of the Crystallites in Polycrystalline Materials

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Abstract

In the most general case the orientation distribution of crystals in a polycrystalline sample is to be described by a function of orthogonal transformations which splits up into two functions of rotations corresponding to right- and left-handed crystals. The properties of these functions are influenced by crystal and sample symmetry. The rotational subgroup of crystal symmetry leads to symmetry relations which may be written in the form of selection rules. Elements of the second kind of the crystal symmetry give rise to a determinability condition, according to which the texture function may be split into a part $\tilde{f}(g)$ which can be determined from polycrystal diffraction experiments and a part $\tilde{\tilde{f}}(g)$ which cannot. The determinability condition may take on three different forms according to whether the crystal symmetry contains a centre of inversion, a mirror plane or a $\bar{4}$ inversion axis. In the case of normal scattering the Laue symmetry is to be considered instead of the true crystal symmetry. The sample symmetry is to be described by a black–white or Shubnikov group containing four kinds of elements which give rise to four kinds of symmetry conditions in the function $f(g)$. The sample symmetry may be a conventional one consisting of one-to-one relationships between crystal orientations. It may, however, also be a non-conventional one defined by an integral relation between an infinite number of crystal orientations.

1. Introduction

The texture of a polycrystalline material is defined as the orientation distribution function $f(g)$ which describes the orientation density or relative frequency f of crystallites having the orientation g with respect to the sample coordinate system. The crystal orientation g has usually been defined as a *rotation* which brings the sample coordinate system into coincidence with the crystal coordinate system (or *vice versa*).

This definition of crystal orientation is, however, not general enough since it does not allow one to deal with enantiomorphic crystal classes consisting of right- and left-handed crystal forms. But also in the higher symmetric classes this definition is not sufficient in as far as it does not allow one to take symmetry elements of the second kind of the crystal symmetry *correctly* into account, *i.e.* mirror planes, inversion axes, and the centre of symmetry. It is thus necessary to generalize the definition of crystal orientation to orthogonal

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transformations $\mathscr{O}$ which include also transformations of the second kind transforming a right-handed coordinate system into a left-handed one (Esling, Bunge & Muller, 1980).

A polycrystalline sample may exhibit a symmetry of its own, the statistical sample symmetry, which is independent of crystal symmetry. This symmetry has been described by point symmetry groups (Weissenberg, 1922; Paterson & Weiss, 1961) which establish a statistical equivalence between certain sample directions related to one another by the symmetry elements of these groups (including symmetry elements of the second kind). In consequent pursuance of the generalized concept of crystal orientation, the concept of the statistical sample symmetry needs also to be generalized. The equivalence of two sample directions in the statistical sense must be judged by the ensemble of crystal directions falling into the respective sample direction (the inverse pole figure of this sample direction). In the generalized concept, crystal directions of right-handed and left-handed crystals are to be distinguished although they are crystallographically equivalent (a similar distinction is necessary also in non-enantiomorphic crystals). In the former concept of sample symmetry this difference could not be taken into account. Thus, an additional attribute is introduced in the concept of sample symmetry which may take on one of two values, *i.e.* right or left. This is, exactly, the concept of Shubnikov's black–white groups if one identifies right with white and left with black. A correct description of sample symmetry thus requires Shubnikov groups instead of the usual point symmetry groups (Bunge, Esling & Muller, 1980).

It is the purpose of the present paper to deduce thoroughly the consequences of crystal and sample symmetry on the orientation distribution function with the complete description of crystal orientation by orthogonal transformations instead of rotations only.

It will be shown that symmetry elements of the second kind in the crystal symmetry give rise to a superposition of pole figures, which, in turn, leads to the indeterminability of a certain part of the texture function. This was pointed out for the first time by Matthies (1979) in the specific case of the centre of inversion as a symmetry element of the second kind.

The determinability condition is mathematically identical with the symmetry condition required by certain non-conventional symmetry elements of the sample symmetry. In the former, incomplete, concept of crystal orientation, considering only rotations, these two conditions could not be distinguished. The *determinability* condition in the case of centrosymmetric crystals ($l = 2l'$) was thus assumed to be a *symmetry* condition which is, however, in general not the case.

The fact that part of the distribution function remains indeterminable from polycrystal diffraction experiments leads to a falsification of the true distribution function. In the specific case of centrosymmetry this so-called ghost structure has been extensively studied in the last two years by Matthies (1980, 1981), Matthies & Pospiech (1980), Jura, Lücke & Pospiech (1980) and Lücke, Pospiech, Virnich & Jura (1981).

The 'indeterminable' part of the texture function is not 'absolutely' indeterminable. Four methods have been proposed of how to determine at least an approximation to the indeterminable part. In principle, the indeterminability arises from the superposition of pole figures. It does not occur in individual orientation determinations (Bunge & Esling, 1979*a*,*b*; Wenk, Wagner, Esling & Bunge, 1981). If the distribution function contains zero ranges then the indeterminable part is exactly determined in these ranges and can be extrapolated to the non-zero ranges (Bunge & Esling, 1979*a*,*b*; Esling, Bechler-Ferry & Bunge, 1981). If it is assumed that the true texture function is a superposition of a low number of Gaussian components then a fixed relationship exists between the indeterminable and the determinable part (Jura *et al.*, 1980; Lücke *et al.*, 1981) from which the indeterminable part can be obtained. And, finally, the specific indeterminability introduced by Friedel's law can be circumvented by the use of anomalous scattering (Bunge & Esling, 1981). It is, however, not the purpose of the present paper to deal with the specific features of the ghost structure, nor will the question be discussed how the indeterminability can be overcome.

2. The orientation distribution function

In order to describe crystal orientations in a polycrystalline sample we fix a rectangular, right-handed coordinate system K_A in the sample. Another coordinate system K_B is fixed in each crystal. It consists of equivalent crystal directions in all crystals. The orientation of a crystal is defined by the orthogonal transformation o which transforms K_A into K_B

$$K_B = o K_A. \tag{1}$$

The transformations o form a group, the orthogonal group $\mathscr{O}(3)$. If K_B is right-handed, the same as K_A, then the transformation o is a rotation g. If K_B is left-handed then o is an element of the second kind which may be considered as the product of a rotation g and the centre of inversion, gI. The orthogonal group thus consists of the elements

$$\mathscr{O}(3) = \{o\} = \{g, gI\}. \tag{2}$$

Accordingly, (1) can take the two forms

$$K_B = gK_A \tag{3}$$

$$K_B = gIK_A = gK_A^I, \tag{4}$$

where K_A^I is a left-handed sample coordinate system which consists of the opposite directions compared with the ones forming K_A:

$$K_A^I = IK_A. \qquad (5)$$

The rotation g may be represented as the product of three successive rotations about the Z,X,Z axes, respectively, *i.e.* the Euler angles

$$g = g^Z(\varphi_2)\, g^X(\phi)\, g^Z(\varphi_1) = \{\varphi_1,\phi,\varphi_2\}. \qquad (6)$$

There is no continuous path in the group $\mathscr{O}(3)$ leading from an element g to an element of the second kind gI, *i.e.* the orthogonal group $\mathscr{O}(3)$ consists of two connected components. The orientation distribution function thus splits into two separate functions (Esling, Bunge & Muller, 1980) describing the orientation distribution of the right- and left-handed crystals respectively:

$$f(\mathscr{g})\begin{cases} = f(g) = M^R f^R(g) \\ = f(gI) = M^L f^L(g), \end{cases} \qquad (7)$$

where the factors M^R and M^L describe the relative amount of right-handed and left-handed crystals respectively.

$$M^R + M^L = 1. \qquad (8)$$

Both functions are normalized according to the condition

$$\int f^{R,L}(g)\,\mathrm{d}g = 1. \qquad (9)$$

Where R,L means that a relation of this type holds for f^R as well as for f^L.

The orientation distribution function can be developed into a series of generalized spherical harmonics

$$f^{R,L}(g) = \sum_{l=0}^{\infty}\sum_{m=-l}^{+l}\sum_{n=-l}^{+l} C_l^{R,Lmn}\, T_l^{mn}(g). \qquad (10)$$

3. The axis distribution function

A crystal direction $\mathbf{h}$ is defined by its coordinates $h_1 h_2 h_3$ in K_B which may be written

$$\mathbf{h} = \{h_1 h_2 h_3\}\, K_B. \qquad (11)$$

Similarly, for a sample direction,

$$\mathbf{y} = \{y_1 y_2 y_3\}\, K_A. \qquad (12)$$

The corresponding sample direction in the left-handed sample system K_A^I is

$$\mathbf{y}^I = \{y_1 y_2 y_3\}\, K_A^I. \qquad (13)$$

It is related to the direction $\mathbf{y}$ by

$$\mathbf{y}^I = I\mathbf{y} = -\mathbf{y}. \qquad (14)$$

The axis distribution function $A(\mathbf{h},\mathbf{y})$ is defined by the integral of the texture function over all crystal orientations for which a crystal direction $\mathbf{h}$ is parallel to the sample direction $\mathbf{y}$ (Bunge, 1969). A function of this type can be defined for right- and left-handed crystals

$$A^{R,L}(\mathbf{h},\mathbf{y}) = \frac{1}{2\pi}\int_{\mathbf{h}\parallel\mathbf{y}} f^{R,L}(g)\,\mathrm{d}g. \qquad (15)$$

This function obeys the relation

$$A^{R,L}(-\mathbf{h},-\mathbf{y}) = A^{R,L}(\mathbf{h},\mathbf{y}). \qquad (16)$$

It has been shown (Bunge, 1969) that the axis distribution function of right-handed crystals can be expressed by the coefficients C_l^{mn} of (10) by

$$A^R(\mathbf{h},\mathbf{y}) = \sum_l\sum_m\sum_n \frac{4\pi}{2l+1}\, C_l^{Rmn}\, k_l^{*m}(\mathbf{h})\, k_l^n(\mathbf{y}). \qquad (17)$$

The identical relation holds for left-handed crystals if the sample direction $\mathbf{y}$ is replaced by the 'left-handed' direction $\mathbf{y}^I$. If it is, however, to be referred to the right-handed sample coordinate system K_A it is (Bunge, Esling & Muller, 1980)

$$A^L(\mathbf{h},\mathbf{y}) = \sum_l\sum_m\sum_n \frac{4\pi}{2l+1}\,(-1)^l\, C_l^{Lmn}\, k_l^{*m}(\mathbf{h})\, k_l^n(\mathbf{y}). \qquad (18)$$

If we do not want to, or if in a considered problem it is not possible to, distinguish between the direction $\mathbf{h}$ of a right-handed crystal and the direction $\mathbf{h}$ of a left-handed crystal falling into the sample direction $\mathbf{y}$, we define a superposed axis distribution function

$$\bar{A}(\mathbf{h},\mathbf{y}) = M^R A^R(\mathbf{h},\mathbf{y}) + M^L A^L(\mathbf{h},\mathbf{y}). \qquad (19)$$

4. Crystal symmetry

The crystals may exhibit symmetries. This means that an orthogonal transformation $\mathscr{g}^c$ brings the crystal lattice into a position indistinguishable from the first one. Two crystal directions $\mathbf{h}$ and $\mathbf{h}'$ related by a symmetry operation are symmetrically equivalent, which we designate by the symbol $\equiv$,

$$\mathbf{h}' = \mathscr{g}^c\,\mathbf{h}, \quad \mathbf{h}' \equiv \mathbf{h}. \qquad (20)$$

Similarly, the two coordinate systems K_B and K_B' are symmetrically equivalent

$$K_B' = \mathscr{g}^c K_B, \quad K_B' \equiv K_B. \qquad (21)$$

The coordinate system K_B' is related to K_A by the orientation $\mathscr{g}'$ which is equivalent to $\mathscr{g}$

$$K_B' = \mathscr{g}^c K_B = \mathscr{g}^c\, \mathscr{g} K_A = \mathscr{g}' K_A \qquad (22)$$

$$\mathscr{g}' = \mathscr{g}^c\, \mathscr{g}, \qquad \mathscr{g}' \equiv \mathscr{g}. \tag{23}$$

The symmetry elements $\mathscr{g}^c$ form a group, the point symmetry group of the crystal. They may be of the first or second kind

$$\mathscr{G}^c = \{\mathscr{g}^c\} = \{g^c, \bar{g}^c I\}. \tag{24}$$

The equivalence of $\mathscr{g}$ and $\mathscr{g}'$ in (23) requires the invariance of the function f with respect to the transformation $\mathscr{g}^c$

$$f(\mathscr{g}^c\, \mathscr{g}) = f(\mathscr{g}). \tag{25}$$

Since both $\mathscr{g}$ and $\mathscr{g}^c$ may be of the first or second kind, (25) splits into the four relations

$$f^R(g^c g) = f^R(g),\ f^L(g^c g) = f^L(g), \tag{26}$$

$$f^L(\bar{g}^c g) = f^R(g),\ f^R(\bar{g}^c g) = f^L(g), \tag{27}$$

$$M^R = M^L = \tfrac{1}{2}.$$

Similarly, it is required for the axis distribution functions

$$A^R(g^c\mathbf{h},\mathbf{y}) = A^R(\mathbf{h},\mathbf{y}),$$

$$A^L(g^c\mathbf{h},\mathbf{y}) = A^L(\mathbf{h},\mathbf{y}), \tag{28}$$

$$A^L(-\bar{g}^c\mathbf{h},\mathbf{y}) = A^R(\mathbf{h},\mathbf{y}),$$

$$A^R(-\bar{g}^c\mathbf{h},\mathbf{y}) = A^L(\mathbf{h},\mathbf{y}). \tag{29}$$

5. The determinability condition

In polycrystal diffraction experiments symmetrically equivalent crystal directions, falling into the same sample direction $\mathbf{y}$, cannot be distinguished. Hence, we can define a symmetrized function which is the mean value over all functions obtained by the application of all crystal symmetry elements. It is to be noted that the inversion centre relating a right-handed crystal to a left-handed one is not an element of crystal symmetry although the corresponding right- and left-handed crystal directions are indistinguishable in polycrystal experiments, too. In the case that the crystal symmetry group $\mathscr{G}^c$ contains only elements of the first kind we have thus to define symmetrized functions for the right- and left-handed crystals separately:

$$\tilde{A}^{R,L}(\mathbf{h},\mathbf{y}) = \frac{1}{N}\sum_{\{g^c\}} A^{R,L}(g^c\mathbf{h},\mathbf{y}), \tag{30}$$

where N is the order of the group $\mathscr{G}^c$, *i.e.* the number of its elements.

Owing to the symmetries of the orientation distribution function (26), it follows with (28)

$$\tilde{A}^{R,L}(\mathbf{h},\mathbf{y}) = A^{R,L}(\mathbf{h},\mathbf{y}). \tag{31}$$

If the crystal symmetry contains elements of the second kind, then there is only one crystal form which may be considered as right- and left-handed at the same time. In this case the symmetrized function must be defined

$$\tilde{A}(\mathbf{h},\mathbf{y}) = \tfrac{1}{2}[\tilde{A}^R(\mathbf{h},\mathbf{y}) + \tilde{A}^L(\mathbf{h},\mathbf{y})]. \tag{32}$$

With (30) this may be written

$$\tilde{A}(\mathbf{h},\mathbf{y}) = \frac{1}{2N'}\left[\sum_{\{g^c\}} A^R(g^c\mathbf{h},\mathbf{y}) + \sum_{\{g^c\}} A^L(g^c\mathbf{h},\mathbf{y})\right], \tag{33}$$

where now N' is the order of the rotational subgroup of the group of crystal symmetry.

Because of (28) this is

$$\tilde{A}(\mathbf{h},\mathbf{y}) = \tfrac{1}{2}[A^R(\mathbf{h},\mathbf{y}) + A^L(\mathbf{h},\mathbf{y})]. \tag{34}$$

Because of (29) A^L is related to A^R by any one of the elements of the second kind $\bar{g}^c I$:

$$\tilde{A}(\mathbf{h},\mathbf{y}) = \tfrac{1}{2}[A^R(\mathbf{h},\mathbf{y}) + A^R(-\bar{g}^c\mathbf{h},\mathbf{y})]. \tag{35}$$

The elements of the second kind of the crystal symmetry are inversion axes of crystallographic type, *i.e.*

$$\bar{g}^c I = \bar{1}, \bar{2}, \bar{3}, \bar{4}, \bar{6}. \tag{36}$$

Since $\bar{3}$ contains $\bar{1}$ and $\bar{6}$ contains $\bar{2}$ only the three elements of the second kind

$$\bar{g}^c I = \bar{1}, \bar{2}, \bar{4} = I, m, \bar{4} \tag{37}$$

are to be considered. It is further to be mentioned that $\bar{4}$ contains a twofold axis. Let us further assume that the axes in (37) are parallel to the Z axis of the crystal coordinate system K_B. (This restriction can later on easily be dropped by a transformation of the coordinate system K_B.) The rotations $\bar{g}^c$ can then be written

$$\bar{g}^c = \left\{\frac{2\pi}{K}, 0, 0\right\}, \quad K = 1, 2, 4. \tag{38}$$

If the crystal direction $\mathbf{h}$ is expressed by its spherical polar coordinates $\phi\beta$ instead of the Cartesian coordinates $h_1\, h_2\, h_3$ in K_B,

$$\mathbf{h} = \{\phi, \beta\}\, K_B, \tag{39}$$

then the direction $-\bar{g}^c\mathbf{h}$ has the polar coordinates

$$-\bar{g}^c\mathbf{h} = \left\{\pi - \phi, \beta + \pi + \frac{2\pi}{K}\right\} K_B. \tag{40}$$

With the definition of the spherical harmonics

$$k_l^m(\mathbf{h}) = \frac{1}{\sqrt{2\pi}}\, \bar{P}_l^m(\phi)\, e^{im\beta} \tag{41}$$

and the relation

$$\bar{P}_l^m(\pi - \phi) = (-1)^{l+m}\, \bar{P}_l^m(\phi), \tag{42}$$

this leads to

$$k_l^m(-\bar{g}^c\,\mathbf{h}) = (-1)^{l+2m/K}\,k_l^m(\mathbf{h}). \qquad (43)$$

With (35) and (17) one obtains

$$\tilde{A}(\mathbf{h},\mathbf{y}) = \sum_l \sum_m \sum_n \frac{4\pi}{2l+1}\, C_l^{Rmn}\,\tfrac{1}{2}[1 + (-1)^{l+2m/K}] \times k_l^{*m}(\mathbf{h})\,k_l^n(\mathbf{y}). \qquad (44)$$

If we put

$$\tilde{C}_l^{mn} = C_l^{Rmn}\,\tfrac{1}{2}[1 + (-1)^{l+2m/K}], \qquad (45)$$

(44) becomes

$$\tilde{A}(\mathbf{h},\mathbf{y}) = \sum_l \sum_m \sum_n \frac{4\pi}{2l+1}\, \tilde{C}_l^{mn}\, k_l^{*m}(\mathbf{h})\,k_l^n(\mathbf{y}). \qquad (46)$$

Equation (46) has the same form as (17). Hence, only the coefficients $\tilde{C}_l^{mn}$ can be obtained from experimentally determined axis distribution functions $\tilde{A}(\mathbf{h},\mathbf{y})$. They define a function

$$\tilde{f}(g) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \sum_{n=-l}^{+l} \tilde{C}_l^{mn}\, T_l^{mn}(g) \qquad (47)$$

which can be obtained directly from polycrystal diffraction experiments (*cf.*, however, Friedel's law). The function

$$\tilde{\tilde{f}}(g) = f(g) - \tilde{f}(g) \qquad (48)$$

cannot be obtained directly since the coefficients $\tilde{\tilde{C}}_l^{mn}$ belonging to this function are being multiplied by the factor in square brackets in (45) which is in this case zero. The function $\tilde{\tilde{f}}(g)$ is thus 'blotted out' because of the superposition of the axis distribution functions belonging to crystallographically equivalent crystal directions. In the various crystal symmetry groups, the determinability condition takes on the form given in Table 1. It must be mentioned that the indeterminability of the part $\tilde{\tilde{f}}(g)$ is a consequence of polycrystal diffraction. A condition of such a kind does not occur if $f(g)$ is determined from individual crystal orientation measurements (Bunge & Esling, 1979*a*,*b*).

The indeterminability of the part $\tilde{\tilde{f}}(g)$ is not always an absolute one as one might conclude from (45). As a distribution function of crystal orientations, the function $f(g)$ cannot be negative

$$f(g) = \tilde{f}(g) + \tilde{\tilde{f}}(g) \geq 0. \qquad (49)$$

If one knows – as is frequently the case – that $f(g)$ must be zero in certain ranges Z^0 of orientations g, then $\tilde{\tilde{f}}(g)$ is known in these places, too, because of the relation

$$\tilde{\tilde{f}}(g) = -\tilde{f}(g) \quad \text{in } Z^0. \qquad (50)$$

It has been shown that the knowledge of $\tilde{\tilde{f}}(g)$ in Z^0 can be used to calculate an approximation to $\tilde{\tilde{f}}(g)$ in the whole orientation space (Bunge & Esling, 1979*a*,*b*). In the case of ideal textures consisting only of one orientation g_0 and the range spread about it, the zero range is so large that (50) allows one to determine $\tilde{\tilde{f}}(g)$ to a high degree of accuracy. But also in more realistic cases such as the rolling texture of copper the zero range seems to be large enough practically to overcome the indeterminability condition (Esling, Bechler-Ferry & Bunge, 1981).

It is further noted that the diffraction process usually adds an inversion centre to the crystal symmetry, the effective crystal symmetry thus being the Laue symmetry. This is known as Friedel's law. As is seen in Table 1, Friedel's law always adds the determinability condition l = even. In the case of centrosymmetric crystals this does not change anything. In the case $\bar{2}$ the additional condition m = even occurs which corresponds to a twofold axis in the direction of $\bar{2}$ and in the case $\bar{4}$ the additional condition $m/2$ = even corresponds to a fourfold axis which are both not present in the crystal symmetries.

Friedel's law does, however, not hold in certain cases of anomalous scattering in the vicinity of an absorption edge of one of the elements in the crystal structure. In these cases it will be possible to obtain terms with odd values of l in the series expansion of polycrystal experiments and only in these cases is it possible to obtain the complete 'determinable' part $\tilde{f}(g)$ according to Table 1 (Bunge & Esling, 1981).

Finally, it must be mentioned that the crystal direction **h** of a right-handed crystal is indistinguishable from the same direction of a left-handed crystal. If

Table 1. *The determinability condition for the three types of symmetry elements of the second kind*

Crystal symmetry

	$\bar{1} = I$	$\bar{2} = m$	$\bar{4}$	
Determinable part $\tilde{f}(g)$	l	$l + m$	$l + \frac{m}{2}$	even
Indeterminable part $\tilde{\tilde{f}}(g)$				odd

Crystal symmetry groups

C_i	$\bar{1}$	C_s	m	S_4	$\bar{4}$
C_{2h}	$2/m$	C_{2v}	mm	D_{2d}	$\bar{4}2m$
D_{2h}	mmm	D_{2d}	$\bar{4}2m$	T_d	$\bar{4}3m$
C_{4h}	$4/m$	C_{4v}	$4mm$		
D_{4h}	$4/mmm$	C_{3v}	$3m$		
C_{3i}	$\bar{3}$	C_{3h}	$\bar{6}$		
D_{3d}	$\bar{3}m$	D_{3h}	$\bar{6}2m$		
C_{6h}	$6/m$	C_{6v}	$6mm$		
D_{6h}	$6/mmm$	T_d	$\bar{4}3m$		
T_h	$m3$				
O_h	$m3m$				

the sample contains right- and left-handed crystals at the same time, as will be the normal case in the enantiomorphic crystal classes, then only the axis distribution function $\bar{A}(\mathbf{h},\mathbf{y})$ of (19) can be measured. With (17) and (18) this leads to

$$\bar{A}(\mathbf{h},\mathbf{y}) = \sum_{l}\sum_{m}\sum_{n} \frac{4\pi}{2l+1}\, \bar{C}_l^{mn}\, k_l^{*m}(\mathbf{h})\, k_l^{n}(\mathbf{y}) \qquad (51)$$

with

$$\bar{C}_l^{mn} = M^R\, C_l^{Rmn} + (-1)^l\, M^L\, C_l^{Lmn}, \qquad (52)$$

which defines a superposed texture of the right- and left-handed crystals

$$\bar{f}(g) = \sum_{l=0}^{\infty}\, \sum_{m=-l}^{+l}\, \sum_{n=-l}^{+l} \bar{C}_l^{mn}\, T_l^{mn}(g), \qquad (53)$$

as has been shown by Bunge, Esling & Muller (1980).

6. Sample symmetry

The question of sample symmetry is more complex than the question of crystal symmetry. It can only be answered in a statistical sense. Two sample directions $\mathbf{y}$ and $\mathbf{y}'$ are said to be equivalent if the same distribution of crystal directions $\mathbf{h}$ falls into them. If we distinguish directions $\mathbf{h}$ of right-handed and left-handed crystals then two kinds of symmetry operations may also be distinguished. Those which relate two sample directions $\mathbf{y}$ and $\mathbf{y}'$ judged by the right-handed crystal directions (or left-handed crystal directions) falling into them and those which relate right-handed directions falling into $\mathbf{y}$ to left-handed ones falling into $\mathbf{y}'$.

$$\mathbf{y}' = \mathscr{g}^s\mathbf{y}, \quad \mathbf{y}' \equiv \mathbf{y}, \qquad (54)$$

$$\mathbf{y}'' = \mathscr{g}'^s\mathbf{y}, \quad \mathbf{y}'' \equiv' \mathbf{y}, \qquad (55)$$

where $\equiv'$ denotes the second type of equivalence. The equivalence relations (54) and (55) are defined by

$$A^R(\mathbf{h}, \mathscr{g}^s\mathbf{y}) = A^R(\mathbf{h},\mathbf{y}),$$

$$A^L(\mathbf{h}, \mathscr{g}^s\mathbf{y}) = A^L(\mathbf{h},\mathbf{y}) \qquad (56)$$

$$A^L(\mathbf{h}, \mathscr{g}'^s\mathbf{y}) = A^R(\mathbf{h},\mathbf{y}),$$

$$A^R(\mathbf{h}, \mathscr{g}'^s\mathbf{y}) = A^L(\mathbf{h},\mathbf{y}), \qquad (57)$$

$$M^R = M^L = \tfrac{1}{2}.$$

The symmetry operations $\mathscr{g}^s$ and $\mathscr{g}'^s$ form a group in which, thus, four types of elements may be distinguished

$$S^s = \left\{\begin{matrix} \mathscr{g}^s \\ \mathscr{g}'^s \end{matrix}\right\} = \left\{\begin{matrix} \boxed{g^s} & \bar{g}^s I \\ g'^s\, 1' & \boxed{\bar{g}'^s\, 1' I} \end{matrix}\right\}, \qquad (58)$$

where $1'$ is a symmetry element which transforms right-handed $\mathbf{h}$ directions into left-handed ones. This group is a black–white or Shubnikov group. The element $1'$ changes, for example, the colour of a point from white into black and *vice versa.* Illustrations of these groups have been given by Shubnikov & Belov (1964) and in the case of sample symmetry by Bunge, Esling & Muller (1980).

6.1. *Conventional symmetry*

Sample symmetry may also be considered in another way. We may assume the *whole sample* to be transformed in a statistical sense by a symmetry operation $\mathscr{g}^p$ in such a way that every crystal in an orientation $\mathscr{g}$ has its counterpart in the orientation $\mathscr{g}\,\mathscr{g}^p$. This crystal has thus the same orientation $\mathscr{g}$ with respect to a transformed sample coordinate system K'_A. It is

$$K'_A = \mathscr{g}^p K_A \quad K'_A \equiv K_A \qquad (59)$$

and

$$K'_B = \mathscr{g}K'_A = \mathscr{g}\,\mathscr{g}^p K_A = \mathscr{g}' K_A, \qquad (60)$$

$$\mathscr{g}' = \mathscr{g}\,\mathscr{g}^p \quad \mathscr{g}' \equiv \mathscr{g}. \qquad (61)$$

These symmetry elements form a normal point symmetry group in which two kinds of elements are to be distinguished

$$\mathscr{G}^p = \{\mathscr{g}^p\} = \{g^p, \bar{g}^p I\}. \qquad (62)$$

This kind of symmetry is completely analogous to the formerly defined crystal symmetry. It requires the symmetry condition

$$f(\mathscr{g}\,\mathscr{g}^p) = f(\mathscr{g}), \qquad (63)$$

which reads in detail

$$f^R(gg^p) = f^R(g),$$

$$f^L(gg^p) = f^L(g), \qquad (64)$$

$$f^L(g\bar{g}^p) = f^R(g),$$

$$f^R(g\bar{g}^p) = f^L(g), \qquad (65)$$

$$M^R = M^L = \tfrac{1}{2}.$$

From these conditions the corresponding ones for the axis distribution functions can be deduced

$$A^R(\mathbf{h}, g^p\mathbf{y}) = A^R(\mathbf{h},\mathbf{y}),$$

$$A^L(\mathbf{h}, g^p\mathbf{y}) = A^L(\mathbf{h},\mathbf{y}), \qquad (66)$$

$$A^L(\mathbf{h}, -\bar{g}^p\mathbf{y}) = A^R(\mathbf{h},\mathbf{y}),$$

$$A^R(\mathbf{h}, -\bar{g}^p\mathbf{y}) = A^L(\mathbf{h},\mathbf{y}). \qquad (67)$$

By comparison with (56) and (57), it follows that

$$g^p = g^s, \quad \bar{g}^p = \bar{g}'^s. \tag{68}$$

The symmetry defined by (54)–(57) is thus more general than the one defined by (59)–(61). The latter may be called conventional sample symmetry. The conventional symmetry elements are encased by dashed lines in (58).

7. Symmetry conditions

7.1. *Crystal symmetry*

7.1.1. *Elements of the first kind.* The symmetry rotations g^c of the crystal symmetry (24) are assumed to be rotations about the Z axis of K_B (this specification can later on be dropped by a transformation of the coordinate system K_B).

$$g^c = \left\{ \frac{2\pi}{K}, 0, 0 \right\} \quad K = 1, 2, 3, 4, 6, \tag{69}$$

with g of (6) it is

$$g^c g = \left\{ \varphi_1, \phi, \varphi_2 + \frac{2\pi}{K} \right\}; \tag{70}$$

with the definition of the generalized spherical harmonics

$$T_l^{mn}(\varphi_1\, \phi\, \varphi_2) = e^{im\varphi_2} P_l^{mn}(\phi)\, e^{in\varphi_1}, \tag{71}$$

it follows that

$$T_l^{mn}(g^c g) = T_l^{mn}(g)\, e^{im(2\pi/K)} = T_l^{mn}(g)\, (-1)^{2m/K}. \tag{72}$$

The symmetry condition (26) can be written

$$f^{R,L}(g^c g) - f^{R,L}(g) = 0. \tag{73}$$

With the series expansion (10) this becomes

$$\sum_l \sum_m \sum_n C_l^{R,Lmn} [T_l^{mn}(g^c g) - T_l^{mn}(g)] = 0 \tag{74}$$

and with (72)

$$\sum_l \sum_m \sum_n C_l^{R,Lmn}\, T_l^{mn}(g)\, [(-1)^{2m/K} - 1] = 0. \tag{75}$$

From this it follows that

$$C_l^{R,Lmn} = 0 \quad \text{for } m \neq Km', \tag{76}$$
$$m' = 1, 2, 3, \ldots, \quad K = 1, 2, 3, 4, 6.$$

7.1.2. *Elements of the second kind.* For symmetry elements of the second kind, (27) can be written

$$f^{L,R}(\bar{g}^c g) - f^{R,L}(g) = 0, \quad M^R = M^L = \tfrac{1}{2}, \tag{77}$$

from which follows

$$\sum_l \sum_m \sum_n [C_l^{L,Rmn} (-1)^{2m/K} - C_l^{R,Lmn}]\, T_l^{mn}(g) = 0 \tag{78}$$

and this requires

$$C_l^{L,Rmn} = (-1)^{2m/K} C_l^{R,Lmn}, \quad K = 1, 2, 4. \tag{79}$$

In the case $K = 4$ the inversion axis $\bar{4}$ contains a twofold axis. Hence m is even and the exponent in (79) is an integer.

7.2. *Sample symmetry*

We assume the elements of sample symmetry to be rotations about the Z axis of K_A:

$$g^s = \left\{ 0, 0, \frac{2\pi}{K} \right\}, \quad K = 1, 2, 3, \ldots, \infty. \tag{80}$$

(Symmetry elements of sample symmetry need not be crystallographic rotations.) With (6) we obtain

$$g g^s = \left\{ \varphi_1 + \frac{2\pi}{K}, \phi, \varphi_2 \right\}. \tag{81}$$

Similar to (72) one finds

$$T_l^{mn}(g g^s) = (-1)^{2n/K}\, T_l^{mn}(g). \tag{82}$$

7.2.1. *Conventional symmetry elements.* The symmetry condition (64) can be written

$$f^{R,L}(g g^s) - f^{R,L}(g) = 0, \tag{83}$$

from which follows in complete analogy to (74)–(76)

$$C_l^{R,Lmn} = 0 \quad \text{for } n \neq Kn', \tag{84}$$
$$n' = 1, 2, 3, \ldots, \quad K = 1, 2, 3, \ldots, \infty.$$

The symmetry elements of the second kind $\bar{g}'^s I 1'$ require the condition (65) which may be written

$$f^{L,R}(g \bar{g}'^s) - f^{R,L}(g) = 0, \tag{85}$$
$$M^R = M^L = \tfrac{1}{2}.$$

In complete analogy to (77)–(79) this yields the condition

$$C_l^{L,Rmn} = (-1)^{2n/K} C_l^{R,Lmn} \tag{86}$$
$$K = 1, 2, 4K', \ldots, \infty.$$

Elements of the second kind of the sample symmetry need not be crystallographic ones. Inversion axes of the type $2(2K' + 1)$ contain mirror planes $m = \bar{2}$ and those of the type $2K' + 1$ contain $I = \bar{1}$. Hence, axes of these types need not be considered separately. An inversion axis of the type $4K'$ contains a rotation axis of the type $2K'$. The index n in (86) must, therefore, be a multiple of $2K'$ so that the exponent $2n/K'$ is an integer.

7.2.2. *Non-conventional symmetry elements.* The non-conventional symmetry elements $\bar{g}^s I$, (58), are defined by (56) which can be written in the form

$$A^{R,L}(\mathbf{h}, -\bar{g}^s\,\mathbf{y}) - A^{R,L}(\mathbf{h},\mathbf{y}) = 0. \tag{87}$$

With the series expansion (17) this can be written

$$\sum_l \sum_m \sum_n \frac{4\pi}{2l+1} C_l^{R,Lmn}\, k_l^{*m}(\mathbf{h}) \times [k_l^n(-\bar{g}^s\,\mathbf{y}) - k_l^n(\mathbf{y})] = 0 \tag{88}$$

and, with (43),

$$\sum_l \sum_m \sum_n \frac{4\pi}{2l+1} C_l^{R,Lmn}\, k_l^{*m}(\mathbf{h})\, k_l^n(\mathbf{y}) \times [(-1)^{l+2n/K} - 1] = 0, \tag{89}$$

from which follows

$$C_l^{R,Lmn} = 0 \quad \text{for } l + \frac{2n}{K} \text{ odd}, \tag{90}$$

$$K = 1, 2, 4K', \ldots, \infty.$$

Finally, it follows for the non-conventional symmetry elements $g'^s\,1'$ with (57)

$$A^{L,R}(\mathbf{h}, g'^s\,\mathbf{y}) - A^{R,L}(\mathbf{h},\mathbf{y}) = 0, \tag{91}$$

$$M^R = M^L = \tfrac{1}{2}.$$

With the series expansions (17) and (18) one obtains

$$\sum_l \sum_m \sum_n \frac{4\pi}{2l+1} k_l^{*m}(\mathbf{h})\, [C_l^{L,Rmn}\, k_l^n(g'^s\,\mathbf{y}) - (-1)^l\, C_l^{R,Lmn}\, k_l^n(\mathbf{y})] = 0, \tag{92}$$

from which follows

$$\sum_l \sum_m \sum_n \frac{4\pi}{2l+1} k_l^{*m}(\mathbf{h})\, k_l^n(\mathbf{y})\, [C_l^{L,Rmn}(-1)^{2n/K} - (-1)^l\, C_l^{R,Lmn}] = 0. \tag{93}$$

This requires

$$C_l^{L,Rmn} = (-1)^{l+2n/K}\, C_l^{R,Lmn}, \tag{94}$$

$$K = 1, 2, 3, \ldots, \infty.$$

The symmetry conditions, including the determinability condition, are summarized in Table 2.

7.2.3. *Axial symmetry* (*fibre textures*). It has already been mentioned that the sample symmetry does not need to be a crystallographic symmetry, *i.e.* the order K of the axes is not restricted to the values 1, 2, 3, 4, 6. In the specific case of axial symmetry (fibre textures) K is infinite.

The symmetry elements g^s of (58) (pure rotations) require the symmetry condition (84) which reads in this specific case

$$C_l^{R,Lmn} = 0 \quad \text{for } n \neq 0. \tag{95}$$

Table 2. *The symmetry conditions and the determinability condition for the various kinds of crystal and sample symmetry*

Crystal symmetry

	g^c $(K = 1, 2, 3, 4, 6)$	$\bar{g}^c\,I$ $(K = 1, 2, 4)$
Symmetry condition	$m = Km'$	$C^{L,R} = (-1)^{2m/K}\, C^{R,L}$ $\quad M^L = M^R = \frac{1}{2}$
Determinability condition		$1 + \frac{2m}{K}$ even

Sample symmetry

Conventional		Non-conventional	
g^s $(K = 1, 2, 3, \ldots, \infty)$	$\bar{g}'^s\,1'\,I$ $(K = 1, 2, 4K', \ldots, \infty)$	$\bar{g}^s\,I$ $(K = 1, 2, 4K', \ldots, \infty)$	$g'^s\,1'$ $(K = 1, 2, 3, \ldots, \infty)$
$n = Kn'$	$C^{L,R} = (-1)^{2n/K}\, C^{R,L}$ $M^L = M^R = \frac{1}{2}$	$l + \frac{2n}{K}$ even	$C^{L,R} = (-1)^{l+2n/K}\, C^{R,L}$ $M^L = M^R = \frac{1}{2}$
axial symmetry	$n = 0$ $C^{L,R} = C^{R,L}$ $M^L = M^R = \frac{1}{2}$	l even	$C^{L,R} = (-1)^l\, C^{R,L}$ $M^L = M^R = \frac{1}{2}$
∞	$\frac{\infty}{m'}$	$\frac{\infty}{m}$	∞'

Because

$$I^2 = 1'^2 = 1 \tag{96}$$

the second powers of the other symmetry elements $\bar{g}^s I$, $g'^s\, 1'$, $\bar{g}'^s\, 1'\, I$ of (58) are pure rotations too and, in fact, they are rotations of infinite order. Hence, the symmetry condition (95) must be fulfilled in all cases of axial symmetry. In these cases the sample symmetry condition takes on the forms given in the last line of Table 2 (*cf.* Bunge, Esling & Muller, 1980).

In the case $n = 0$, the generalized spherical harmonics (71) are independent of the angle φ_1. They are, but for a constant factor, identical with the surface spherical harmonics (41). It is

$$T_l^{m0}(\phi,\varphi_2) = \left(\frac{4\pi}{2l+1}\right)^{1/2} e^{-l(\pi/4)}\, k_l^m(\phi,\varphi_2). \tag{97}$$

The orientation distribution functions (10) can then be developed into a series of surface spherical harmonics

$$f^{R,L}(\phi,\varphi_2) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} C_l^{R,Lm}\, k_l^m(\phi,\varphi_2), \tag{98}$$

depending on two angular variables only. This case is usually treated separately, although it is completely contained in the general formulae taking into account the axis of infinite order.

7.3. *Combination of crystal and sample symmetry*

The sample symmetry element $\bar{g}'^s\, 1'\, I$ (Table 2) establishes a relationship between the coefficients of the functions in the right- and left-handed crystal coordinate systems. If, furthermore, the crystal symmetry is non-enantiomorphic, *i.e.* it contains an element of the second kind $\bar{g}^c I$, then there is another relationship between these two types of coefficients. One thus obtains by combining these two relations

$$C^{L,R} = (-1)^{2n/K_s}\,(-1)^{2m/K_c}\, C^{L,R}, \tag{99}$$

where K_c and K_s are the constants K of Table 2 for crystal and sample symmetry respectively.

Equation (99) can be written

$$C^{L,R}[1 - (-1)^{2n/K_s + 2m/K_c}] = 0. \tag{100}$$

It follows from (100) that

$$C_l^{L,Rmn} = 0 \tag{101}$$

for

$$\frac{2n}{K_s} + \frac{2m}{K_c}\ \text{odd}. \tag{102}$$

Similarly, one obtains in the case of the sample symmetry $g'^s\, 1'$ and crystal symmetry $\bar{g}^c I$,

$$C_l^{L,Rmn} = 0 \tag{103}$$

for

$$l + \frac{2n}{K_s} + \frac{2m}{K_c}\ \text{odd}. \tag{104}$$

Hence, combination of the four sample-symmetry cases with the two crystal-symmetry cases of Table 2 gives the combined symmetry conditions of Table 3.

7.4. *Change of the coordinate system*

In §§ 7.1 and 7.2, it has been assumed that the symmetry rotations g^c, g^s and g'^s and the rotations $\bar{g}^c$, $\bar{g}^s$ and $\bar{g}'^s$ contained in the symmetry elements of the second kind are parallel to the Z axes of the sample and crystal coordinate systems K_A and K_B, respectively. If this assumption is to be dropped we have only to introduce new sample and crystal coordinate systems. Let the new sample coordinate system be

$$K'_A = g_l K_A, \tag{105}$$

Table 3. *Symmetry conditions according to the combination of crystal and sample symmetry*

Sample symmetry

	Conventional		Non-conventional	
Crystal symmetry	g^s	$\bar{g}'^s\, 1'\, I$	$\bar{g}^s I$	$g'^{s1'}$
g^c	$m = K_c m'$ $n = K_s n'$ $C^{L,R} = (-1)^{2m/K_c}\, C^{R,L}$	$m = K_c m'$ $C^{L,R} = (-1)^{2n/K_s}\, C^{R,L}$ $C^{L,R} = (-1)^{2m/K_c}\, C^{R,L}$	$m = K_c m'$ $l + \frac{2n}{K_s}$ even $C^{L,R} = (-1)^{2m/K_c}\, C^{R,L}$	$m = K_c m'$ $C^{L,R} = (-1)^{l+2n/K_s}\, C^{R,L}$ $C^{L,R} = (-1)^{2m/K_c}\, C^{R,L}$
$\bar{g}^c I$	$n = K_s n'$	$C^{L,R} = (-1)^{2n/K_s}\, C^{R,L}$ $\frac{2n}{K_s} + \frac{2m}{K_c}$ even	$l + \frac{2n}{K_s}$ even	$C^{L,R} = (-1)^{l+2n/K_s}\, C^{R,L}$ $l + \frac{2n}{K_s} + \frac{2m}{K_c}$ even

then the orientation g' with respect to this system is defined by

$$K_B = g' K_A' = g' g_l K_A = g K_A, \qquad (106)$$

from which follows

$$g = g' g_l, \quad g' = g g_l^{-1}. \qquad (107)$$

The orientation distribution functions (10) can be written in this system

$$f'^{R,L}(g') = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \sum_{s=-l}^{+l} C_l'^{R,Lms} T_l^{ms}(g'). \qquad (108)$$

This may be expressed in terms of the rotation g

$$f^{R,L}(g) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \sum_{s=-l}^{+l} C_l'^{R,Lms} T_l^{ms}(g g_l^{-1}). \qquad (109)$$

The application of the addition theorem gives

$$f^{R,L}(g) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \sum_{s=-l}^{+l} \sum_{n=-l}^{+l} C_l'^{R,Lms} T_l^{mn}(g)\, T_l^{ns}(g_l^{-1}). \qquad (110)$$

This can be written

$$f^{R,L}(g) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \sum_{n=-l}^{+l} C_l^{R,Lmn} T_l^{mn}(g) \qquad (111)$$

with the coefficients

$$C_l^{R,Lmn} = \sum_{s=-l}^{+l} C_l'^{R,Lms} T_l^{ns}(g_l^{-1}). \qquad (112)$$

If the symmetry conditions of the sample symmetry (Table 2) are known in the system K_A, *i.e.* in terms of the coefficients $C_l^{R,Lmn}$, then (112) gives the transformation of these conditions into the new sample coordinate system K_A' in which the symmetry axes are not parallel to the Z axis.

Similarly, one obtains for a new crystal coordinate system

$$K_B' = g_j K_B. \qquad (113)$$

The crystal orientation with respect to this system is given by

$$K_B' = g_j K_B = g_j g K_A = g' K_A \qquad (114)$$

with

$$g' = g_j g, \quad g = g_j^{-1} g'. \qquad (115)$$

In complete analogy with (108)–(112), one obtains the transformation relation of the coefficients

$$C_l^{R,Lmn} = \sum_{s=-l}^{+l} C_l'^{R,Lsn} T_l^{sm}(g_j). \qquad (116)$$

With an appropriate choice of the rotations g_l and g_j for each symmetry element the symmetry conditions (Table 2) can be transformed into the most general form.

8. Conclusions

The orientation of a crystal in a polycrystalline sample may be described by an orthogonal transformation which transforms a sample coordinate system K_A into a crystal coordinate system K_B. This transformation may either be a rotation or an operation of the second kind which changes a right-handed coordinate system into a left-handed one and *vice versa*. The orientation distribution function of crystals (the texture) thus consists of two functions of rotations, *i.e.* the orientation distribution functions of right-handed and left-handed crystal coordinate systems, respectively.

With respect to orientation distribution functions, two different types of symmetries are to be taken into account, the crystal symmetry and the statistical sample symmetry.

The rotational subgroup of crystal symmetry gives rise to symmetry conditions imposed upon the orientation distribution functions of the right-handed crystals and of the left-handed crystals, respectively.

The elements of the second kind of crystal symmetry require a relationship between the two distribution functions such that in fact only one of them is really needed, corresponding to only one crystal form which is, at the same time, right-handed and left-handed. They do not, however, impose further symmetry conditions on this function.

The elements of the second kind of crystal symmetry lead to a superposition of pole figures. As a consequence of this, only one part of the texture function, $\tilde{f}(g)$, is determinable by polycrystal diffraction experiments, the remaining part, $\tilde{\tilde{f}}(g)$, is ‘invisible’ in all pole figures because of the specific properties of the ‘projection’ by which the symmetrized pole figure is obtained from the orientation distribution function.

The determinability condition may take on three different forms, namely l = even, $l + m$ = even, $l + m/2$ = even, according to whether the crystal symmetry contains the inversion centre, a mirror plane, or a $\bar{4}$ axis as an element of the second kind. In the case of normal scattering Friedel’s law always adds an inversion centre.

The sample symmetry may be considered in two different ways. In the *conventional* way, every crystal may have its symmetrical counterpart (in a statistical sense) in one or more symmetrically-related orientations. These may be right-handed crystals or left-handed ones as well. Symmetry is thus defined by a *one-to-one* relationship between crystal orientations.

In a more general sense, sample symmetry can be defined by individual crystal directions falling into symmetrically-related sample directions. It is thus possible, for example, to have a centrosymmetrical sample consisting of only right-handed crystals of an enantiomorphic crystal symmetry. This *non-conventional* type of sample symmetry cannot be obtained by a one-to-one relationship between crystals in two different orientations. It rather requires an integral relationship between an *infinite* number of crystal orientations.

An exhaustive description of all possible kinds of sample symmetry cannot be given by a normal point symmetry group. It rather requires black–white Shubnikov groups.

The specific case of centrosymmetric crystals is especially important in texture analysis in metallurgy since the basic metals, crystallizing in f.c.c., b.c.c. and h.c.p. lattices, are centrosymmetric. The determinability condition l = even for this case has attracted much attention in the last few years.

The non-centrosymmetric crystal classes are more important in mineralogical and geological problems. Applications of the present considerations to non-centrosymmetrical crystal classes have not yet been reported. Investigations in this direction are presently being carried out and will be published elsewhere.

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Numerical Structure Factor Calculation of Orientationally Disordered Molecules

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Abstract

The structure factor of librating or orientationally disordered molecules with isotropic Gaussian distribution functions is calculated exactly by numerical integration. The computer program with an example is described. The results are compared with approximation methods which correspond to a cumulant expansion of the structure factor. The application to the refinement of the plastic phases of C_2Cl_6 and SF_6 is shown. The influence of anharmonic distributions is considered. The method is compared to the analysis with spherical cubic harmonics.

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1. Introduction

There are many crystal structures which contain groups of atoms where the binding forces within a group are higher than those to the surrounding atoms. Such groups are called 'rigid molecules' if the internal vibration frequencies are considerably higher than the external or lattice mode frequencies. With this definition charged groups are included also.

For rigid molecules the thermal motion can be treated in a good approximation as the motion of a rigid body. But, also, disorder which is not of thermal origin can then be regarded as positional or orientation-