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Symmetries in Texture Analysis

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Abstract

It is shown that a comprehensive symmetry description in polycrystalline bodies needs black-white point groups rather than the usual (one-colour) groups that are sufficient for single crystals.

1. Introduction

Crystalline solids such as metals, ceramics or natural rocks usually exhibit a polycrystalline structure, *i.e.* they consist of small crystallites of the same crystal structure but with different orientations of their crystallographic axes. The orientation distribution of the crystallites is called the *texture* of the materials. If all crystal orientations are equally frequent, the material is then said to be macroscopically isotropic, *i.e.* its properties are the same in all directions. If, however, different orientations are present with different relative frequencies, the anisotropies of the crystallites will, in general, not cancel each other and the material will be macroscopically anisotropic, *i.e.* its physical properties will be different when measured in different sample directions. In the latter case, symmetries may be observed in the directional dependence of the properties according to the specific features of the orientation distribution function. This type of symmetry has been called *sample symmetry* and it should be kept distinct from crystal symmetry. The sample symmetry in rolled metal sheets, for example, is determined by the symmetry of the production process, *i.e.* the geometry of the roll gap by which the material

has been shaped. This is an orthorhombic symmetry and the same *type* of symmetry is found in materials with different crystal structure and crystal symmetry, *e.g.* in cubic, hexagonal, tetragonal metals. (The details of the orientation distribution of the crystallites are, of course, different in these cases whereas the type of sample symmetry is the same.)

The purpose of this paper is to show that sample symmetries in polycrystalline materials can arise in two different ways, either by one-to-one relations between individual crystal orientations (conventional symmetry operations) or by certain integral relations taken over a continuous manifold of orientations (non-conventional symmetry operations). The non-conventional symmetry operations can occur in addition to the conventional ones, thus requiring an extension of the conventional point-symmetry groups for polycrystals (Bunge, Esling & Muller, 1980). The most efficient description of this extension is that of black-white groups considered for the first time by Heesch (1930), Shubnikov (1951) and Niggli & Wondratschek (1960).

It should be mentioned that black-white symmetries have been considered in connection with textures by Shubnikov (1958), Shubnikov, Sheludev, Konstantinova & Silvestrova (1958), Shubnikov & Belov (1964), but in a completely different sense. In these cases crystals having an additional black-white property were considered, whereas in the present paper the black-white notation is being used in order to describe certain properties of the orientation distribution of single-coloured crystals. A comprehensive

discussion of the symmetries in textured materials has also been given by Paterson & Weiss (1961). But this work does not consider, any more than the other ones mentioned above, the possible existence of non-conventional symmetry operations.

2. Crystal symmetry

We consider a coordinate system K_B in each crystal-lite, which is assumed to be made up of the same basis vectors. The position of the origin of K_B is considered irrelevant. A crystal direction can then be characterized by a unit vector \mathbf{h} with components h_1, h_2, h_3 with respect to K_B . A crystal symmetry operation (point symmetry) is defined by a unitary transformation of crystal directions, which relates a transformed direction \mathbf{h}' to any crystal direction \mathbf{h} ,

$$h'_i = a_{ij}h_j, \quad (1)$$

such that \mathbf{h} and \mathbf{h}' are crystallographically *equivalent*, which may be symbolized by

$$\mathbf{h}' \circ \rightarrow \mathbf{h}. \quad (2)$$

The space transformation (1) and the equivalence relation (2) define together a symmetry operation in the space of the crystal directions \mathbf{h} . The symmetry operation may be of first or second kind according to whether the determinant $|a_{ij}|$ is +1 or -1. The crystal symmetry, made up of the totality of symmetry operations (1) and (2), is described by one of the 32 crystallographic point groups.

3. Sample symmetry

We now consider a polycrystalline sample and fix another coordinate system K_A in it. A sample direction can then be defined by a unit vector \mathbf{y} with the components y_1, y_2, y_3 . In order to define the sample symmetry in the same way as the definition of crystal symmetry, (1), (2), we should first define what we mean when we say that two sample directions \mathbf{y} and \mathbf{y}' are *equivalent*. Because of the statistical nature of a polycrystal this question can only be answered in a statistical sense. Two sample directions \mathbf{y} and \mathbf{y}' are said to be equivalent if the same 'amount' of crystal directions \mathbf{h} fall into them. The totality of crystal directions \mathbf{h} coinciding with a fixed sample direction \mathbf{y} is defined by a distribution function.

$$R_y(\mathbf{h}) = (1/V) dV/d\Omega, \quad (3)$$

which describes the volume fraction dV/V of crystal-lites, the crystal direction \mathbf{h} of which is parallel to the fixed sample direction \mathbf{y} within the solid angular element $d\Omega$, *i.e.* the surface element on the pole sphere. This distribution function (as a function of \mathbf{h}) is called the *inverse pole figure* of the sample direction \mathbf{y} . The inverse pole figure may be represented for example by level lines in a stereographic

projection on a certain crystal plane as is shown, for example, in Fig. 1. The equivalence of two sample directions \mathbf{y} and \mathbf{y}' is then defined by the identity of their inverse pole figures.

We first consider crystals without symmetry, *i.e.* crystals belonging to class 1. This is an enantiomorphic class, *i.e.* right- and left-handed crystals may be present in the material. In the most general case the amounts M^R and M^L of the right- and left-handed fractions may be different and this may apply to the respective textures, too. Correspondingly, we also have to consider two inverse pole figures, *i.e.* the ones of the right- and of the left-handed fraction. An equivalence of two sample directions \mathbf{y} and \mathbf{y}' is then obtained if the inverse pole figures are identical in the two directions.

$$R_y^R(\mathbf{h}) = R_{y'}^R(\mathbf{h}), \quad R_y^L(\mathbf{h}) = R_{y'}^L(\mathbf{h}) \quad (4)$$

as shown in Fig. 1(a) (equivalence of first mode).

The crystal lattice of the right-handed crystals can be transformed into that of the left-handed crystals by a unitary transformation, similar to (1) with $|a_{ik}| = -1$. In this way a crystal direction \mathbf{h}^L in the left-handed crystal is related uniquely to the corresponding direction \mathbf{h}^R in the right-handed crystal. The two directions are crystallographically equivalent in the same sense as symmetry-related directions \mathbf{h} and \mathbf{h}' within a crystal, *i.e.* they are equivalent in the sense of (2). The equivalence of two sample directions \mathbf{y} and \mathbf{y}' can then be defined in a generalized way. Two sample directions \mathbf{y} and \mathbf{y}' are also said to be equivalent (equivalence of second mode) if the same 'amount'

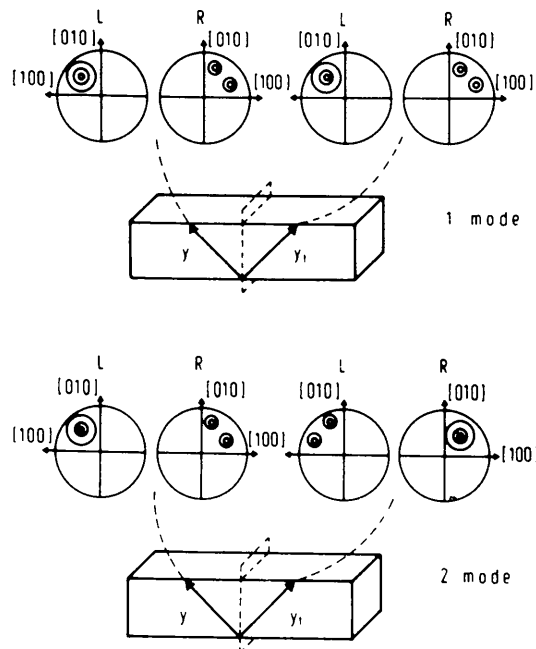


Fig. 1. Two modes of equivalences of two sample directions defined by the inverse pole figures of right- and left-hand crystals.

of *equivalent* crystal directions h^R and h^L respectively falls into them. In this case the inverse pole figures are 'cross related':

$$R_y^L(\mathbf{h}) = R_y^R(\mathbf{h}), \quad R_y^R(\mathbf{h}) = R_y^L(\mathbf{h}), \quad (5)$$

as is shown in Fig. 1(b). Using these relations we define a symmetry operation of the sample symmetry by a unitary transformation of sample directions

$$y'_i = a_{ij}y_j, \quad (6)$$

which may be of first or second kind, according to whether the determinant $|a_{ij}|$ is +1 or -1, in complete analogy to the definition of (1) in the space of crystal directions. At the same time, we may however have either of two different equivalence relations, which we symbolize as

$$\begin{aligned} \mathbf{y}' &\overset{\curvearrowright}{\sim} \mathbf{y} \text{ first mode;} \\ \mathbf{y}' &\overset{\times}{\sim} \mathbf{y} \text{ second mode.} \end{aligned} \quad (7)$$

The sample symmetry operations can thus be classified in four categories S, S', \bar{S}, \bar{S}' according to Fig. 2. The symmetry operations S and \bar{S} (corresponding to the equivalence of first mode) belong to one of the classical point-symmetry groups, and since we are not dealing with crystal symmetry here, they are not restricted to the crystallographic groups. The symmetry operations S' and \bar{S}' (corresponding to the equivalence of second mode) exchange the right- and left-handed inverse pole figures. The product of two such operations is an operation of first mode. This can be symbolized by a colour change from black to white or *vice versa*. The sample symmetry in a polycrystalline sample is thus correctly described by a black-white point group.

The description of sample symmetries by black-white point groups has been suggested by Bunge, Esling & Muller (1980) who discussed symmetry properties of orientation distribution functions of tex-

tured materials. The symmetry conditions in these functions corresponding to the various symmetry classes were considered later on in detail by Bunge, Esling & Muller (1981), Bunge (1982*b*), and Matthies & Helming (1982). In these papers it was also shown that the classical point groups (including the non-crystallographic ones) are not sufficient to cover all possible sample symmetries because of the existence of two different equivalence relations (7). In Fig. 3, four sample symmetries are considered, as an example, corresponding to twofold axes and twofold inversion axes, *i.e.* mirror planes. Three different sample directions are represented in order to elucidate the change from a right-handed to a left-handed arrangement of these directions by symmetry operations of the second kind. This change is to be kept distinct from the change from black to white according to the second mode of equivalence. Fig. 3 thus represents an example of the four categories of sample symmetries defined in Fig. 2. A further example will be detailed in Fig. 10.

4. Symmetries of pole figures

In Fig. 1 inverse pole figures were used to define the equivalence of two sample directions. The (direct) pole figures are more often used in texture analysis. They represent the distribution of one fixed crystal direction \mathbf{h} over the variable sample directions \mathbf{y}

$$P_h(\mathbf{y}) = (1/V) dV/d\Omega, \quad (8)$$

where dV/V is the volume fraction of crystals having their crystal direction \mathbf{h} parallel to the sample directions \mathbf{y} within the solid angular element $d\Omega$. The only

		equivalence of sample directions	
		1. mode	2. mode
Geometrical symmetry operations relating sample directions			
	1. kind	S	S'
	2. kind	\bar{S}	\bar{S}'

Fig. 2. Sample symmetry operations can be divided into four categories according to the mode of equivalence and the kind of symmetry operation.

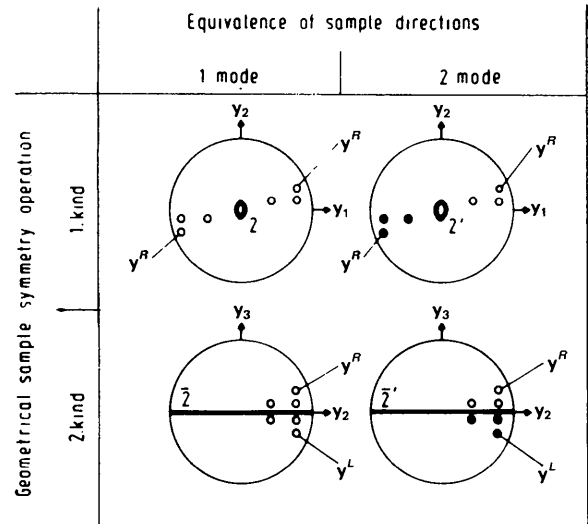


Fig. 3. Sample symmetry operations of the first and second kind relating sample directions that are equivalent according to the first or second mode of equivalence. All points are in the upper hemisphere.

difference with respect to the inverse pole figure (3) lies in the variabilities of the two directions h and y . Whereas in (3) the sample direction y is fixed and the crystal direction h is continuously variable, the opposite is true in the (direct) pole figure (8). Pole figures may be represented by equi-level lines drawn in a stereographic projection (projected onto a specific sample plane) as shown in Fig. 4. Again, we have to consider the distribution of the corresponding crystal direction of the right-handed and left-handed crystals. The symmetries in Fig. 4 are the same as those in Fig. 3. As can be seen in Fig. 4, the symmetry operations *without* a dash operate within each pole figure (right and left) whereas the ones *with* a dash include a transition from the right-handed to the left-handed pole figure. They are thus colour-changing operations.

5. Conventional and non-conventional symmetry operations

In the general case we are dealing with continuous orientation distributions, which we assume to be built up by an infinite (or at least a very large) number of crystallites. The symmetry operations of the sample symmetry considered in the preceding sections are defined on the basis of the totality of crystal directions coinciding with the considered sample directions, irrespective of which individual crystallites these crystal directions belong to. In fact, every crystallite contributes to any chosen sample direction with one particular crystal direction. The symmetry operations of the sample symmetry, so defined, are integral relations over all crystallites of the sample.

We may, however, wonder if, in specific cases, these integral conditions can be fulfilled in a simple way

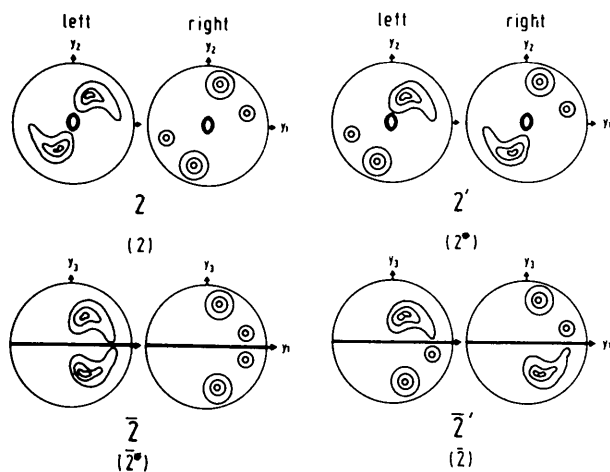


Fig. 4. The sample symmetries 2 , $2'$, $\bar{2}$, $\bar{2}'$ as seen in the pole figures of the right- and left-handed crystals (the symmetry symbols in parentheses correspond to an alternative notation that is explained in § 7).

by only a few crystallites. As is to be seen in Fig. 5, this is possible, for instance, with the symmetries 2 and $\bar{2}'$ of Fig. 3. The symmetry 2 can be fulfilled by putting two right-handed crystals into orientations related by the twofold axis so that their directions h_2^R fall into the two sample directions y^R of Fig. 3. Similarly, the symmetry $\bar{2}'$ can be easily fulfilled by putting a right- and a left-handed crystal into mirror-related orientations. One easily sees that the required symmetry relations are then automatically fulfilled *for all other sample directions*, of which three are explicitly shown in Figs. 3 and 5. If one tries to fulfil the remaining two symmetry cases of Fig. 3 in a similar way with only two crystals, one sees that this is not possible. Indeed, the handedness of the sample directions required by the geometrical part of the symmetry operation (6) (same handedness in $2'$, opposite handedness in $\bar{2}$) does not correspond to the handedness of crystal directions (indicated by black and white), which are to be parallel to these directions. Symmetry operations of this type have thus been assumed to be contradictory in their very definition.

The contradiction disappears, however, if one admits (corresponding to the integral definition of the sample symmetry operation) that the crystal directions h_1, h_2, h_3 required in the three neighbouring sample directions (Fig. 3) need not necessarily belong to one and the same crystallite. They may belong, for example, to three different crystallites. Of course, in this case, the symmetry will be violated in other sample directions but this can be taken care of by adding further crystals. This leads to a never-ending procedure, which cannot possibly be imagined beyond a few steps. The question is then whether it

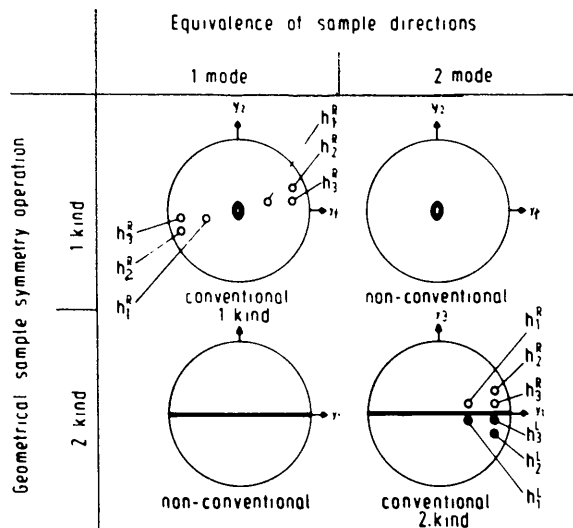


Fig. 5. The conventional sample symmetries of the first and second kinds can be fulfilled by a low number of crystals, e.g. two crystals in the present case (stereographic projection in the sample coordinate system).

is possible to fulfil these symmetry cases by an *infinite* number crystals, *i.e.* by *true* orientation distribution functions (the two crystals assumed as an example in the conventional symmetry cases may also be considered as 'distribution functions', but they are very specific functions having a δ character). If we assume genuine orientation distribution functions of right-handed and left-handed crystals of class 1 and if we consider the most general case then the pole distributions of the right-handed directions \mathbf{h}^R and of the left-handed \mathbf{h}^L may each be chosen independently and deliberately. They may be chosen specifically in the forms shown in the upper-right or the lower-left cases of Fig. 4, *i.e.* with the symmetries $2'$ and $\bar{2}$ assumed in these figures. The sample symmetries required in Fig. 3 were based on the equality of *inverse* pole figures of the corresponding sample directions. They are thus fulfilled if the symmetries of Fig. 4 are likewise fulfilled for *all* pole figures of all possible crystal directions \mathbf{h}^R and \mathbf{h}^L . The symmetries $\bar{2}$ and $2'$ of Fig. 3 (and similar cases) will then be called *non-conventional* symmetries.

6. Are non-conventional symmetry operations really possible?

The various pole figures belonging to different crystal directions \mathbf{h} are not independent of each other. They are related to the orientation distribution function of the crystallites. The question whether the non-conventional symmetries in Fig. 4 can be fulfilled for *all* pole figures is thus the question of the possible existence of an appropriate orientation distribution function. If we deal with enantiomorphic crystals we have to consider two orientation distribution functions $f^R(g)$ and $f^L(g)$.

$$\begin{aligned} f^R(g) &= (1/V^R) dV^R/dg; \\ f^L(g) &= (1/V^L) dV^L/dg, \end{aligned} \quad (9)$$

where g stands for the crystal orientation represented, for example, by three Eulerian angles, dV^R/V^R and dV^L/V^L are the volume fractions of right- and left-handed crystals, respectively, having the orientation g within the orientation element dg , *i.e.* a volume element in the three-dimensional orientation space. The pole figures are related to the orientation distribution functions by the integral relations (Esling, 1981; Bunge, 1982b).

$$\begin{aligned} P_{\mathbf{h}}^R(\mathbf{y}) &= (2\pi)^{-1} \int f^R(g) d\gamma, \\ P_{\mathbf{h}}^L(\mathbf{y}) &= (2\pi)^{-1} \int f^L(g) d\gamma, \end{aligned} \quad (10)$$

where the integrals are taken over all those crystal orientations for which the crystal direction \mathbf{h}^R (or \mathbf{h}^L) is parallel to the sample direction \mathbf{y} . The above-mentioned question can easily be answered if the functions f^R and f^L are represented by series (*cf.*

Bunge, 1982a; Bunge & Esling, 1982a)

$$\begin{aligned} f^R(g) &= \sum_{lmn} {}^R C_1^{mn} T_1^{mn}(g); \\ f^L(g) &= \sum_{lmn} {}^L C_1^{mn} T_1^{mn}(g), \end{aligned} \quad (11)$$

where $T_1^{mn}(g)$ are harmonic functions. The two textures are thus completely represented by the two sets of coefficients ${}^R C_1^{mn}$ and ${}^L C_1^{mn}$. It has been shown that the pole figures can also be expressed in terms of these coefficients:

$$\begin{aligned} P_{\mathbf{h}}^R(\mathbf{y}) &= \sum_{lmn} (4\pi)(2l+1)^{-1} {}^R C_1^{mn} k_l^{*m}(\mathbf{h}) k_l^n(\mathbf{y}); \\ P_{\mathbf{h}}^L(\mathbf{y}) &= \sum_{lmn} (4\pi)(2l+1)^{-1} (-1)^{lL} {}^L C_1^{mn} k_l^{*m}(\mathbf{h}) k_l^n(\mathbf{y}); \end{aligned} \quad (12)$$

where k_l^n are spherical harmonics that have the form

$$k_l^n(\mathbf{y}) = k_l^n(\alpha, \beta) = (2\pi)^{-1/2} \bar{P}_l^n(\alpha) \exp(in\beta) \quad (13)$$

where $\bar{P}_l^n(\alpha)$ are the associated Legendre functions. The asterisk refers to the conjugate complex quantity. The functions (13) have the twofold symmetry axis required in Fig. 4 if n is even and they have a mirror plane if $l+n$ is even (see for example Bunge, 1982a).

In order to fulfil the sample symmetry $\bar{2}$ of Fig. 4 it is necessary that *all* pole figures, right- and left-handed, are each mirror symmetrical. This entails that the coefficients of the functions $k_l^n(\mathbf{y})$ in (12) should be zero for those indices that violate the mirror conditions $l+n$ even:

$$\sum_m {}^R C_1^{mn} k_l^{*m}(\mathbf{h}) = \sum_m {}^L C_1^{mn} k_l^{*m}(\mathbf{h}) = 0 \quad \text{for } l+n \text{ odd.} \quad (14)$$

Since (14) must be fulfilled for *all* crystal directions \mathbf{h} , it implies that all texture coefficients vanish for $l+n$ odd. This is the necessary and sufficient condition for the non-conventional sample symmetry $\bar{2}$ to be fulfilled.

The symmetry $2'$ in Fig. 4 requires a relationship between the right-handed and left-handed pole figures, (12). If we designate by \mathbf{y} and \mathbf{y}' two sample directions related by the twofold axis, the relationship $P_{\mathbf{h}}^L(\mathbf{y}') = P_{\mathbf{h}}^R(\mathbf{y})$ must be fulfilled. According to (13) it is $k_l^n(\mathbf{y}') = (-1)^n k_l^n(\mathbf{y})$, which requires with (12)

$$\sum_m {}^L C_1^{mn} k_l^{*m}(\mathbf{h}) = (-1)^{l+n} \sum_m {}^R C_1^{mn} k_l^{*m}(\mathbf{h}). \quad (15)$$

Equation (15) must be valid for all pole figures \mathbf{h} , thus leading to the final condition

$${}^L C_1^{mn} = (-1)^{l+n} {}^R C_1^{mn}. \quad (16)$$

In this case, the symmetry is obtained by a relation between right- and left-handed crystals. This requires equal volume fractions of the crystal forms ($M^R = M^L = 1/2$). Considerations similar to those applying to the two cases of non-conventional symmetries in

Table 1. *Symmetry conditions expressed in terms of the series coefficients for the symmetry cases of Fig. 4*

$$\begin{array}{l} {}^R C_l^{mn} = {}^L C_l^{mn} = 0 \\ \text{for} \\ n \text{ odd} \\ \bar{2} \end{array} \quad \begin{array}{l} {}^L C_l^{mn} = (-1)^{l+n} {}^R C_l^{mn} \\ M^L = M^R \\ 2' \end{array}$$

$$\begin{array}{l} {}^R C_l^{mn} = {}^L C_l^{mn} = 0 \\ \text{for} \\ l+n \text{ odd} \\ \bar{2} \end{array} \quad \begin{array}{l} {}^L C_l^{mn} = (-1)^n {}^R C_l^{mn} \\ M^L = M^R \\ \bar{2}' \end{array}$$

Fig. 4 also hold for the conventional ones $\bar{2}$ and $2'$. The symmetry conditions summarized in Table 1 are thus obtained.

For a certain function $f(\mathbf{g})$ to be a possible orientation distribution function, the latter must be positive. (There cannot be less than no crystal in any orientation.) Hence, the positivity conditions $f^R(\mathbf{g}) \geq 0$ and $f^L(\mathbf{g}) \geq 0$ must be added to the symmetry conditions of Table 1. This restricts the allowable ranges of the coefficients ${}^R C_l^{mn}$ and ${}^L C_l^{mn}$. It is, however, easy to see that a distribution function of the type

$$f(\mathbf{g}) = 1 + C_l^{mn} T_l^{mn}(\mathbf{g}), \quad |C_l^{mn}| \leq 1, \quad (17)$$

is always positive (Bunge & Esling, 1982*b*). Distribution functions of the type (17) with coefficients ${}^L C_l^{mn}$ and ${}^R C_l^{mn}$, when chosen to meet the conditions of Table 1, prove the possible existence of non-conventional symmetries such as $\bar{2}$ and $2'$. As was shown in Fig. 5, the conventional sample symmetries can be obtained by adding a crystal of the same or opposite handedness in a symmetrically related orientation to any crystal in any orientation present in the sample. This one-to-one relation can easily be imagined. Non-conventional symmetries can only be built up in truly continuous distribution functions. If we deal with true polycrystals we deal anyway with truly continuous distribution functions, even when dealing with conventional sample symmetries. This considerably reduces the conceptual difference between the two modes of symmetries. The only difference left from this point of view is then that the conventional symmetries are much more easily imagined because of the one-to-one relation between individual crystal orientations. It has been argued that a sample symmetry operation that maintains or changes the handedness of *sample* directions has to have the same effect in the space of *crystal* directions. The above mentioned considerations show, however, that this is not the case. The definition of the sample symmetry is completely independent of the crystal symmetry (with only one exception as we shall see later).

7. An alternative notation of the sample symmetries

As was shown in Fig. 2, sample symmetry operations can be divided into four categories, which were distinguished by two different symbols, a bar and a dash.

The bar denotes a geometrical symmetry operation of the second *kind* and the dash denotes an equivalence relation of the second *mode*, which was also symbolized by a black-white change.

The notation of Fig. 2 is in direct accordance with the symmetries in the pole figures shown in Fig. 4. The symmetry operations of the categories S and \bar{S} in Fig. 2 apply directly to the pole figures of the right-handed and of the left-handed crystal fraction. The operations of the categories S' and \bar{S}' involve a transition from the right-handed pole figure to the left-handed one and *vice versa*. (Each of these pole figures by itself does not exhibit the corresponding symmetry.) The black-white change symbolized by the dash does thus correspond to a jump from one pole figures to the other, which is necessary in order for the geometrical symmetry operation to be fulfilled. On the other hand, the *conventional* sample symmetries of the second kind, *i.e.* the ones that change the handedness of sample directions, do also change the handedness of crystal directions falling into them. In the notation of Fig. 2, these conventional symmetry operations are being denoted in a non-classical way by \bar{S}' , *i.e.* including the dash or black-white change. This has been subject to criticism (Donnay & Donnay, 1982). It has been argued that it must be possible to describe the conventional sample symmetries by the classical notation, *i.e.* without a symbol denoting a colour change. This is indeed possible if one also assigns another colour change to the change of handedness of the sample directions, *i.e.* to the geometrical symmetry operations of the second kind. The conventional symmetry operations S and \bar{S}' of Fig. 2 are then characterized by either no change of handedness and hence no colour change (S) or by change of handedness of the sample as well as the crystal directions (\bar{S}'), *i.e.* by two colour changes that cancel each other. Thus, a colour change remains only in those categories of sample symmetries that change handedness of either sample directions or crystal directions, but not both.

These are the non-conventional categories of sample symmetries. In order to distinguish this notation from the one in Fig. 2, another colour-changing symbol must be used, *e.g.* an asterisk. This leads to a second notation, which is given in Fig. 6. This notation does, however, violate the classical notation of symmetries in the pole figures as is seen in Fig. 4. The conventional mirror symmetry in the right-handed and in the left-handed pole distribution functions (lower left) is then denoted in a nonclassical way, *i.e.* including an asterisk, by $\bar{2}^*$.

Hence, one is bound to violate classical symmetry notations anyway. From the point of view of texture analysis the pole figures may be considered as the fundamental quantities. This gives us preference for the notation of Fig. 4. The 'pure' crystallographer, however, may prefer the notation of Fig. 6 in which

the conventional symmetries are denoted in the classical way.

8. Implications of crystal symmetry

8.1. Symmetries of inverse pole figures

We now admit that the crystals themselves may be symmetric. The texture may then be interpreted in such a way that each crystal is assumed to be split into as many equal parts as there are symmetrically equivalent orientations of the crystal coordinate system. In Fig. 7(a) for example the case of a mirror plane is shown. In this case (symmetry operation of the second kind) one part of the crystal belongs to the volume fraction of the right-handed, the other to that of the left-handed crystals. We can thus keep the definition of the right- and left-handed textures, though with a certain relationship between them in the case of non-enantiomorphic crystals. With this

description of the texture, we still have *two* inverse pole figures for each sample direction though with a certain relationship between them depending on the specific crystal symmetry.

In Fig. 8 the inverse pole figures are shown for the crystal symmetry cases 2, $\bar{2}$ and $\bar{1}$. In the case $\bar{2}$ the crystal direction $[h_1 h_2 h_3]$ in the right-handed crystal coordinate system and hence in the right-handed inverse pole figure is identical with the direction $[h_1 \bar{h}_2 h_3]$ in the left-handed crystal coordinate system and hence in the left-handed inverse pole figure. In the case of the inversion centre $\bar{1}$ the relationship is $[h_1 h_2 h_3]$ equivalent to $[\bar{h}_1 \bar{h}_2 \bar{h}_3]$. The symmetry relationships in the inverse pole figures in these three cases are

$$\begin{aligned} 2 R_y^R(h_1 h_2 h_3) &= R_y^R(\bar{h}_1 \bar{h}_2 h_3), R_y^L(h_1 h_2 h_3) = R_y^L(\bar{h}_1 \bar{h}_2 h_3); \\ \bar{2} R_y^L(h_1 h_2 h_3) &= R_y^R(h_1 \bar{h}_2 h_3); \\ \bar{1} R_y^L(h_1 h_2 h_3) &= R_y^R(\bar{h}_1 \bar{h}_2 \bar{h}_3). \end{aligned} \quad (18)$$

Although the right-handed and left-handed inverse pole figures in the non-enantiomorphic cases are *related* to each other, they are not *identical*. The two definitions of equivalence of *sample directions* (4) and (5), Fig. 1, can thus still be applied. The considerations in § 3 on the definition of the sample symmetry

		equivalence of sample directions	
		1 mode	2 mode
Geometrical symmetry operations relating sample directions	1.kind	S	S*
	2.kind	\bar{S}^*	\bar{S}

Fig. 6. A second notation of sample symmetry operations to be compared with Fig. 2.

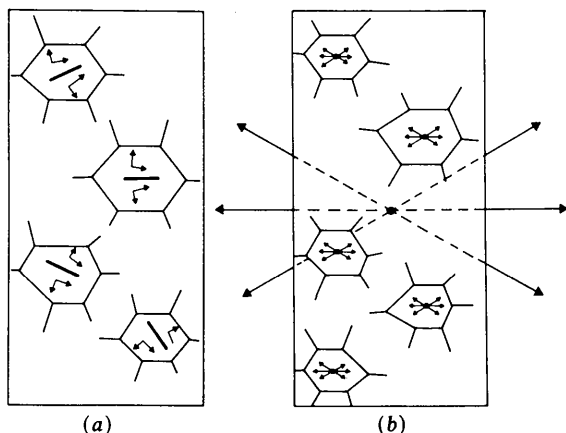


Fig. 7. Crystal and sample symmetry elements. (a) The mirror plane in the crystal symmetry does not imply a mirror plane in the sample symmetry. (b) An inversion centre of the crystal symmetry implies an inversion centre in the sample symmetry.

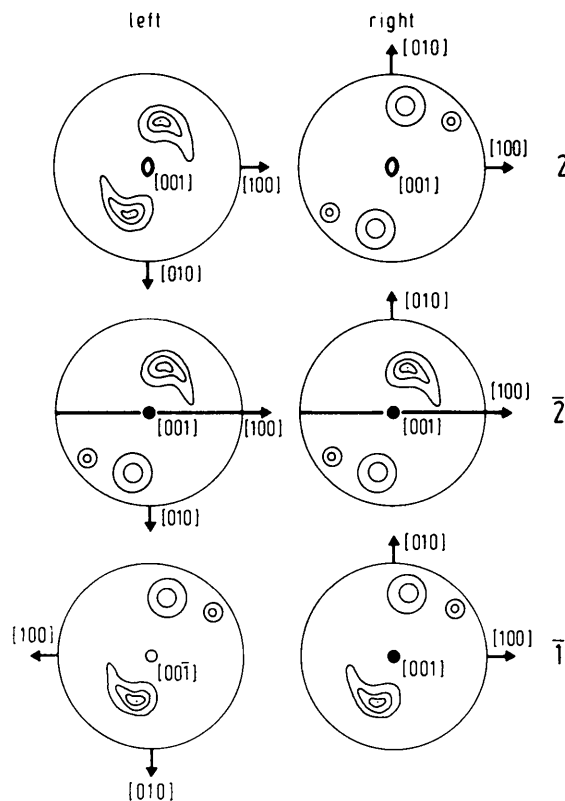


Fig. 8. Right- and left-handed inverse pole figures for the crystal symmetries 2, $\bar{2}$ and $\bar{1}$.

can thus be applied fully also in the cases of non-enantiomorphic crystals (see also Bunge, 1982*b*). It is, of course, also possible in this case to use only *one* crystal coordinate system and hence only *one* inverse pole figure, say the right-handed one. The two equivalence relations (4) and (5) can then be formulated for non-enantiomorphic crystals

$$R_y(\mathbf{h}) = R_{y'}(\mathbf{h}) \text{ mode 1;}$$

$$R_y(\mathbf{h}) = R_{y'}(\mathbf{I.g}\mathbf{h}) \text{ mode 2,} \quad (19)$$

where $\mathbf{I.g}$ is one of the symmetry operations of the second kind of the crystal symmetry.

8.2. Symmetry elements common to crystal and sample symmetry

A crystal symmetry element is, as a rule, oriented differently in the various crystals of a sample, as is shown in Fig. 7(a) for the case of a mirror plane. The mirror plane of the crystal symmetry is thus not an element of the sample symmetry. The same holds for all 'directional' crystal symmetry elements, *i.e.* the n -fold axes and inversion axes with $n \geq 2$. The 'non-directional' inversion centre, on the other hand, is common to all crystals and is thus an element of the sample symmetry as is shown in Fig. 7(b). This is the only (general) case where a symmetry element of the crystal symmetry requires a symmetry element of the sample symmetry.

The various triclinic symmetries are given in the black-white representation in Fig. 9. Sample directions in this figure are represented in stereographic

projection referred to the sample coordinate system in the upper and lower hemispheres. Directions that are equivalent according to the first mode of equivalence are shown in the same colour whereas the second mode of equivalence is indicated by a colour change. This representation corresponds to the

single colour	upper hemisphere	lower hemisphere	1 notation	2 notation	non-convent	centro symm crystals
		0	2	2		
		0	m	m*	+	
		0	2/m	2/m*	+	
grey			2 1'	2 1*	+	
		0	m 1'	m 1*	+	
		0	2/m 1'	2/m 1*	+	+

single colour	upper hemisphere	lower hemisphere	1 notation	2 notation	non-convent	centro symm crystals
		0	1	1		
		0	1	1*	+	
black white			1	1		+
grey			1'	1*	+	
		0	1	1*	+	+

Fig. 9. Triclinic sample symmetries in the black-white representation.

black white	upper hemisphere	lower hemisphere	1 notation	2 notation	non-convent	centro symm crystals
		0	2'	2*	+	
		0	m'	m		
		0	2/m'	2/m		+
		0	2'	2/m*	+	+
		0	2'/m'	2/m*	+	

Fig. 10. Monoclinic sample symmetries in the black-white representation.

first symmetry notation. The first two symmetries are single-colour groups, the third one is a true black-white group and the fourth and fifth ones are grey groups, *i.e.* a point is at the same time black and white.

As is seen in Fig. 9 there are two possible kinds of inversion centres $\bar{1}'$ and $\bar{1}\bar{1}'$ in the sample symmetry that are consistent with an inversion centre in the crystal symmetry. One of these inversion centres is conventional, the other one is non-conventional. A third kind of inversion centre $\bar{1}$ may occur with non-centrosymmetric crystals.

9. Example of specific sample symmetries: the monoclinic symmetries

Since we have referred several times to binary axes 2 and inversion axes $\bar{2}$, the monoclinic black-white groups are shown as examples in Fig. 10. They may be single colour, grey or true black-white. The choice of colours in Figs. 9 and 10 corresponds to the first notation. The second notation is also given in the second column. This notation reflects the conventional and non-conventional symmetries as indicated in the third column. The fourth column again shows the possible symmetry classes for centrosymmetric crystals.

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Simulation of X-ray Traverse Topographs by Means of a Computer

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Abstract

The precision of the numerical algorithm used is the critical factor in computing traverse topographs. The varying-step algorithm allows such a computation. Images have been computed simulating the real experiment, *i.e.* by the addition of the intensities of individual section topographs. Results are in good agreement with experiments: it has been possible to characterize dislocations fully by the study of the fine details of their contrast. This may be of practical interest whenever section topographs cannot be used, as, for instance, in the case of thin crystals.

1. Introduction

Traverse topography is the most popular topographic method since it permits, in one single experiment, the

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study of a large volume of a crystal. However, in most cases, one is restricted to qualitative studies. Section topography allows quantitative measurements but its use is limited: the experiment is rather delicate to perform and becomes impossible in the case of thin crystals where the width of the image is too narrow to see any details.

Authier (1967) attempted to explain the contrast of a traverse topograph as the integration, during the scanning of the crystal, of the direct image of the defect. Applying the kinematical theory he could predict the width of the image. This simplified approach is rather satisfactory (Miltat & Bowen, 1975) but does not permit a full characterisation of the defect.

Quantitative measurements are achieved by the study of the fine details of the contrast of the defect