Classification
Physics Abstracts
81.40E

Description of the texture by distribution functions on the space of orthogonal transformations. Implications on the inversion centre (*)

C. Esling, H. J. Bunge (**) and J. Muller (***)

Laboratoire de Métallurgie Structurale, Ile du Saulcy, 57000 Metz, France

(**) Institut für Metallkunde und Metallphysik der TU Clausthal, F.R.G.

(***) Institut de Mathématiques, rue René Descartes, Strasbourg, France.

(Reçu le 5 mai 1980, révisé le 3 septembre, accepté le 23 septembre 1980)

Résumé. — Dans le cas le plus général, la fonction de distribution des orientations (texture) est une fonction sur l'espace des transformations orthogonales, qui se scinde en un couple de fonctions sur l'espace des rotations. Dans le cas de groupes de symétrie cristalline non énantiomorphes, une seule de ces fonctions est indépendante. La symétrie d'échantillon (notamment la centro-symétrie) peut être réalisée d'une façon triviale et d'une façon non-triviale. La première conduit à des relations entre des valeurs individuelles de fonction, la seconde à des relations intégrales.

Abstract. — In the most general case the orientation distribution function (texture) is a function on the space of orthogonal transformations which splits into a couple of functions on the space of rotations.

In the case of non-enantiomorphic crystal symmetry groups only one of these functions is independent.

Sample symmetry (especially centrosymmetry) can be achieved in a trivial and a non-trivial way. The first one leads to relations between individual functional values the latter one to integral relations.

1. Crystal orientation. — The crystallographic texture of a polycrystalline material is the orientation statistic of its crystallites [1]. The orientation of a crystallite may be described by means of the crystal-fixed reference frame K_b (consisting of crystallographically equivalent directions in each crystal). The reference frame K_b will be referred to a sample fixed reference frame K_a by the orthogonal transformation ϑ which brings K_a into coincidence with K_b

$$K_b = \vartheta \cdot K_a \quad \vartheta \in O(3) \quad (1)$$

where ϑ is an element of the group $O(3)$ of orthogonal transformations in three dimensions. Because of crystal symmetry there may be other reference frames K'_b related to K_b by an element ϑ_b of the crystal symmetry group O_b which are indistinguishable from K_b

$$K'_b = \vartheta_b \cdot K_b \equiv K_b, \quad \vartheta_b \in O_b \quad (2)$$

where $\equiv$ means equivalent or indistinguishable.

Because of the statistical sample symmetry the reference frame K_a will be equivalent with other frames K'_a . This is the case if the orientation statistic is the same from the viewpoints of K_a and K'_a . The two reference systems are related by an operation ϑ_a of the sample symmetry group O_a

$$K'_a = \vartheta_a \cdot K_a \equiv K_a, \quad \vartheta_a \in O_a. \quad (3)$$

Hence, crystal orientation may be described by the double coset of all equivalent orthogonal transformations induced by crystal and sample symmetry.

$$\{ \vartheta_b \cdot \vartheta \cdot \vartheta_a \} \equiv \vartheta. \quad (4)$$

2. The texture function. — The texture function $f(\vartheta)$ is defined by the volume fraction $dV(\vartheta)/V$ of crystals in orientation ϑ , i.e. a function which images the space $O(3)$ of orthogonal transformations onto the space R^+ of real positive numbers which can be symbolically expressed by

$$O(3) \xrightarrow{f} R^+ \\ \vartheta \mapsto f(\vartheta) = \frac{dV(\vartheta)}{V} \quad (5)$$

(*) La version française de cet article a été soumise pour publication aux Comptes Rendus de l'Académie des Sciences.

in such a way that the element $f(\Theta)$ of R^+ corresponds to the element Θ of $O(3)$. Because of the symmetry relation equation (4) the texture function must fulfil the invariance conditions

$$f(\Theta_b \cdot \Theta \cdot \Theta_a) = f(\Theta). \quad (6)$$

An orthogonal transformation Θ is either a rotation g (determinant $+1$) or the product of a rotation (including the identity E) by the inversion centre I (determinant -1). These two kinds of elements cannot be transformed continuously one into the other. Hence, the space $O(3)$ is said to consist of two connexe components containing the elements with determinant $+1$ and -1 respectively. The group $O(3)$ of orthogonal transformations is the cartesian product of the group of rotations $SO(3)$ in three dimensions and the group of the elements E (the identity) and I (the inversion centre).

$$O(3) = SO(3) \times \{E, I\}. \quad (7)$$

The texture function f is thus decomposed into a couple of functions f^r and f^l defined on the space of rotation $SO(3)$ each

$$f(\Theta) = \{f^r(g), f^l(g)\} \quad (8)$$

such that

$$f(\Theta) \begin{cases} = f(g) = f^r(g) & \text{if } \Theta = g \\ = f(g \cdot I) = f(I \cdot g) = f^l(g) & \text{if } \Theta = Ig = gI. \end{cases} \quad (9)$$

If we assume that the sample coordinate system K_a be right-handed, then crystals, the orientation of which is described by a rotation g , are right-handed too. Crystals, the orientation of which is described by an orthogonal transformation Ig (determinant -1) are left-handed. The functions $f^r(g)$ and $f^l(g)$ are thus the distribution functions of the right- and left-handed crystallites respectively.

From equations (8) and (9) it follows immediately that

$$f(I \cdot \Theta) = f(\Theta \cdot I) = \{f^l(g), f^r(g)\}. \quad (10)$$

This means, if each crystal were replaced by its centrosymmetric one or if the sample coordinate system were changed from right-handed to left-handed then the two distribution functions were to be exchanged [2].

3. Sample symmetries and crystal symmetries. — The usual definition of a point symmetry group requires the equivalence of directions only and not of the reference frames (consisting of three correlated directions). The symmetry conditions contained in equations (3), (4), (6) are thus more restrictive than it is usually assumed. In the most general sense we will only require that any sample direction y in the reference

frame K_a be indistinguishable from the corresponding direction y' defined in K'_a . These directions are related by

$$y' = \Theta_a y \quad y' \equiv y. \quad (11)$$

Two sample directions y and y' will be said to be indistinguishable if the distribution of crystal directions h falling into them respectively is the same. Since the crystal orientation Θ is to be described by the three independent parameters whereas a crystal direction h is fixed by only two parameters, the condition $h \parallel y$ will be fulfilled by a one-dimensional manifold of orientations Θ . The distribution of crystal directions h falling into y is thus obtained by an integral over $f(\Theta)$ along a certain path in the space $O(3)$ [3, 4].

$$R_y(h) = \int_{h \parallel y} f(\Theta) d\Theta. \quad (12)$$

The symmetry requirement equation (11) may thus be expressed by

$$\int_{h \parallel y} f(\Theta) d\Theta = \int_{h \parallel \Theta_a y} f(\Theta) d\Theta \quad (13)$$

which must hold for every crystal direction h and every sample direction y .

3.1 THE TRIVIAL SYMMETRY CONDITION. — Equation (13) has a trivial solution which is given by the right-hand invariance of the equivalence relations equations (4) and (6). This means, each crystal in the orientation Θ has its counterpart in the orientation $\Theta\Theta_a$ (or more strictly speaking the two volume fractions are the same). If, for the crystal in Θ it is $h \parallel y$ then for the crystal in $\Theta\Theta_a$ it is according to equation (11) $h \parallel \Theta_a y$. Hence, along with equation (6), equation (13) is necessarily fulfilled which may be called the trivial solution of equation (13).

3.1.1 Centrosymmetry. — In the following we shall consider the special case

$$\Theta_a = I \quad (14)$$

i.e. we examine centrosymmetric sample symmetry.

We will distinguish three types of crystal symmetries :

1) Groups containing rotations only. In these enantiomorphic groups right- and left-handed crystal forms occur.

2) Groups containing the inversion centre I . In these centrosymmetric groups there is only one crystal form which may be described as right- and left-handed at the same time.

3) Groups containing inversion axes i.e. symmetry elements of the type Ig (determinant -1) but not the inversion centre I itself. In these groups, too, there is only one crystal form which may be described as right- and left-handed at the same time.

In case 1 the right invariance of equation (6) requires

$$f(\Theta \cdot \mathbf{I}) = f(\Theta) . \quad (15)$$

Comparison of equations (8) and (10) immediately gives

$$f^l(g) = f^r(g) . \quad (16)$$

A centre of inversion in the sample symmetry thus requires that the two statistics of the right- and left-handed crystals respectively be the same.

In case 2 $\mathbf{I}$ is an element of the crystal symmetry which commutes with every Θ hence it is

$$f(\mathbf{I} \cdot \Theta) = f(\Theta \cdot \mathbf{I}) = f(\Theta) \quad (17)$$

and it follows in the same way

$$f^l(g) = f^r(g) = f(g) . \quad (18)$$

In this case however the two orientation statistics $f^l(g)$ and $f^r(g)$ are not only equal, they are identical since there is only one kind of crystals which can be described in a right-handed as well as a left-handed reference frame (every crystal is its own centrosymmetric counterpart). The distribution of these centrosymmetric crystals is described by only one distribution function $f(g)$.

In case 3 $\mathbf{I}g_b = g_b\mathbf{I}$ is an element of the crystal symmetry which requires according to equation (6)

$$f(\mathbf{I} \cdot g_b \cdot \Theta) = f(g_b \cdot \Theta \cdot \mathbf{I}) = f(\Theta) . \quad (19)$$

It thus follows with equations (8) and (10)

$$f^r(g) = f^l(g_b \cdot g), \quad f^l(g) = f^r(g_b \cdot g) \quad (20)$$

i.e. the left-handed orientation statistic is equal to the right-handed one but at orientations rotated through g_b with respect to each other. This is evident since a crystal can be described as a right-handed one and at the same time as a left-handed one but in a reference frame related to the first one by $\mathbf{I}g_b$. The two parts of equation (20) are evident since with $\mathbf{I}g_b$, also $\mathbf{I}g_b^{-1}$ is an element of the crystal symmetry.

An additional inversion centre as an element of the sample symmetry requires further (equations (19) and (15))

$$f(g_b \cdot \Theta) = f(\Theta) \quad (21)$$

from which follows

$$\begin{aligned} f^r(g_b \cdot g) &= f^r(g) \\ f^l(g_b \cdot g) &= f^l(g) . \end{aligned} \quad (22)$$

The second one of these relations follows necessarily from the first one and equation (20).

3.2 THE NON-TRIVIAL SYMMETRY CONDITION. — Equation (13) which reads in the case $\Theta_a = \mathbf{I}$

$$\int_{\mathbf{h}||\mathbf{y}} f(\Theta) d\Theta = \int_{\mathbf{h}||-\mathbf{y}} f(\Theta) d\Theta \quad (23)$$

has also a non-trivial solution if the right- and left-handed statistics each fulfil the integral relation

$$\begin{aligned} \int_{\mathbf{h}||\mathbf{y}} f^r(g) dg &= \int_{\mathbf{h}||-\mathbf{y}} f^r(g) dg \\ \int_{\mathbf{h}||\mathbf{y}} f^l(g) dg &= \int_{\mathbf{h}||-\mathbf{y}} f^l(g) dg . \end{aligned} \quad (24)$$

These integral relations define a specific class of symmetric functions $\tilde{f}^r(g)$ and $\tilde{f}^l(g)$ among the general functions $f^r(g)$ and $f^l(g)$. (It has been shown elsewhere [2, 4] that this class of functions is characterized by the condition $C_l^m = 0$ for $l = 2l' + 1$ in the series expansion on the basis of generalized spherical harmonics.)

In case 1 of crystal symmetry groups there is no further restriction required. Especially there is no need for a relation between the distribution functions of the right- and left-handed crystals. Equation (23) can thus be fulfilled with $f^l \equiv 0$ i.e. the sample may be centrosymmetric with only right-handed crystals present (or only left-handed ones).

In case 2 the condition equation (18) follows from the crystal symmetry. Since equation (18) is sufficient to fulfil the centrosymmetric sample symmetry, centrosymmetric crystals always give rise to centrosymmetric samples. Nevertheless may also in this case equation (23) be fulfilled.

In case 3 the crystal symmetry gives rise to equation (20) thus only one of the distribution functions f^l and f^r is independent but equation (20) does not imply a centre of inversion in the sample symmetry. Hence, equation (24) offers a possibility for the sample to be centrosymmetric other than the trivial solution equation (23).

References

- [1] BUNGE, H. J., *Mathematische Methoden der Texturanalyse* (Akademie-Verlag, Berlin) 1969.
- [2] BUNGE, H. J., ESLING, C. and MÜLLER, J., submitted to *J. Appl. Crystallogr.*
- [3] MATTHIES, S., *Phys. Status Solidi b* **92** (1979) K135.
- [4] BUNGE, H. J. and ESLING, C., *C. R. Hebd. Séan. Acad. Sci.* **289B** (1979) 163; and BUNGE, H. J. and ESLING, C., *J. Physique Lett.* **40** (1979) L-627.