Textures and Microstructures, 1996, Vol. 25, pp. 205–210
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THE INFLUENCE OF CRYSTAL SYMMETRY ON THE DETERMINATION OF THE ORIENTATION OF ISOLATED TEXTURE COMPONENTS FROM POLE FIGURES

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(Received 20 June 1995)

The explicit relationship between the orientation of isolated texture components and peaks in pole figures is given. With this relationship the influence of triclinic and monoclinic crystal symmetry on the determination of the of isolated texture components is considered. In the special case that the problem is not ill-posed the method of the determination of the orientation of isolated texture components from pole figures is proposed.

KEY WORDS: Orientation of isolated texture components, triclinic crystal symmetry, monoclinic crystal symmetry.

INTRODUCTION

Sharp textures, which only consist of few non-overlapping components, reflected correspondingly sharp in the pole figures (PF) too, are considered. The problem of the determination of the orientation of these components from pole figure data is discussed in the present paper.

The properties of symmetry of the diffraction mechanism (Friedel's law) as well the properties of crystal symmetry can lead to non-uniqueness of the solution of this problem even though the single texture component is available. All possible 32 crystal classes can be subdivided into three types (Bunge, Esling and Muller, 1980; Esling, Bunge and Muller, 1980): 1) groups containing rotations only; 2) groups containing the inversion centre; 3) groups containing inversion axes but not the inversion centre itself. In the cases of types 1) and 2) the orientation of an isolated texture component can be determined from PF wheares for the type 3) it cannot, in principle, be unambiguously determined from PF (Matthies and Helming, 1982).

The problem of the determination of the orientation of isolated texture components from pole figures has been dealt with in the works (Matthies., 1981; Helming., 1993; Helming. *et al.*, 1994). Another way of looking at this problem for the cases of hexagonal (point group D_{6h}), cubic (point group O_h) and trigonal (point group D_3) crystal symmetry was proposed in the papers (Bukharova, Savyolova, 1985; Nikolaev, Savyolova, 1987; Ivanova, Savyolova, 1993). In the present paper it has been developed for the cases of triclinic and monoclinic crystal symmetry.

DESCRIPTION OF THE ORIENTATION OF A CRYSTALLITE

Let K_A be the sample coordinate system and K_B be the crystal coordinate system. The orientation g of the crystallite is defined as the rotation which transforms the sample coordinate system into the crystal one. In particular, it is expressed in terms of the Eulerian angles $g = \{\alpha, \beta, \gamma\}$. In the present paper the sequence of rotations is chosen as follows (Korn, and Korn, 1968):

1) rotation of K_A around the axis Z_A by the angle α,
2) rotation of K'_A around the axis Y'_A by the angle β,
3) rotation of K''_A around the axis Z''_A by the angle γ;

$$0 \leq \alpha,\ \gamma < 2\pi,\ 0 < \beta < \pi.$$

Denote the matrix representation of the orientation g by $T(g)$. $T(g)$ is the transformation matrix for the coordinates $\mathbf{y} = (y^1, y^2, y^3)$ of an arbitrary vector in the sample coordinate system K_A expressed by means of the coordinates $\mathbf{h} = (h^1, h^2, h^3)$ of this vector in the crystal coordinate system K_B (Bunge, 1982):

$$\mathbf{y}' = T(g)\mathbf{h}', \tag{1}$$

where $\mathbf{y}' = \begin{pmatrix} y^1 \\ y^2 \\ y^3 \end{pmatrix}$, $\mathbf{h}' = \begin{pmatrix} h^1 \\ h^2 \\ h^3 \end{pmatrix}$. The matrix $T(g)$ is an orthogonal matrix, $\det T(g) = 1$.

RELATIONSHIP BETWEEN THE ORIENTATION OF ISOLATED TEXTURE COMPONENT AND PEAKS IN 'UNREDUCED' POLE FIGURES IN THE CASE OF TRICLINIC CRYSTAL SYMMETRY

Let 'unreduced' pole figure $P_{\mathbf{h}}(\mathbf{y})$ be pole figure determined with the help of anomalous scattering (Matthies and Helming, 1982). In the case of the triclinic crystal symmetry (group C_1, only one sort of enantiomorphic crystals exists in the sample) a peak at $g = g_o$ in the orientation space provides peaks in the 'unreduced' **PF** $P_{\mathbf{h}_1}(\mathbf{y})$ and $P_{\mathbf{h}_2}(\mathbf{y})$ at $\mathbf{y}_1$ and $\mathbf{y}_2$, respectively:

$$\begin{aligned} \mathbf{y}'_1 &= T(g_o)\mathbf{h}'_1\ . \\ \mathbf{y}'_2 &= T(g_o)\mathbf{h}'_2 \end{aligned} \tag{2}$$

The relation between the vector $\mathbf{h}_3 = [\mathbf{h}_1, \mathbf{h}_2]$ and the vector $\mathbf{y}_3 = [\mathbf{y}_1, \mathbf{y}_2]$ is well-known (see Eq. 1)

$$\mathbf{y}'_3 = T(g_o)\mathbf{h}'_3. \tag{3}$$

The Eq. (2), (3) can be rewritten as the system of vector equations

$$\begin{aligned} \mathbf{y}'_1 &= h_1^1\mathbf{T}_1 + h_1^2\mathbf{T}_2 + h_1^3\mathbf{T}_3 \\ \mathbf{y}'_2 &= h_2^1\mathbf{T}_1 + h_2^2\mathbf{T}_2 + h_2^3\mathbf{T}_3 \\ \mathbf{y}'_3 &= h_3^1\mathbf{T}_1 + h_3^2\mathbf{T}_2 + h_3^3\mathbf{T}_3\ , \end{aligned} \tag{4}$$

where $\mathbf{T}_i$ is the i-column vector of the orientation matrix $T(g_o)$. The determinant of the system of Eg. (4) isn't equal to zero. Hence, Eq.(4) has a unique solution. It is given by the following expression

$$\mathbf{T}_i = \frac{1}{|[\mathbf{h}_1,\ \mathbf{h}_2]|^2} \{[\mathbf{y}_1,\ \mathbf{y}_2]^i[\mathbf{h}_1,\ \mathbf{h}_2]^i + \mathbf{y}'_1\ (h_1^i - h_2^i\ (\mathbf{h}_1,\ \mathbf{h}_2)) + \\ + \mathbf{y}'_2\ (h_2^i - h_1^i\ (\mathbf{h}_1,\ \mathbf{h}_2))\},\quad i = 1,\ 2,\ 3, \tag{5}$$

where $\mathbf{h}_1 = (h_1^1,\ h_1^2,\ h_1^3)$, $[\mathbf{h}_1,\ \mathbf{h}_2]^i$ is the i-coordinate of the vector product of $\mathbf{h}_1$, $\mathbf{h}_2$, $(\mathbf{h}_1,\ \mathbf{h}_2)$ is their scalar product. As an example, assume that $\mathbf{h}_1 = (0,\ 0,\ 1)$ and $\mathbf{h}_2 = (1,\ 0,\ 0)$. Then the orientation matrix is equal to

$$T(g_0) = \begin{pmatrix} y_2^1 & [\mathbf{y}_1,\ \mathbf{y}_2]^1 & y_1^1 \\ y_2^2 & [\mathbf{y}_1,\ \mathbf{y}_2]^2 & y_1^2 \\ y_2^3 & [\mathbf{y}_1,\ \mathbf{y}_2]^3 & y_1^3 \end{pmatrix}. \tag{6}$$

By comparing the matrix elements of the orientation matrix $T(g_0)$, expressed in terms of the Eulerian angles (Korn, and Korn, 1968), with the corresponding ones of Eq. (5) one obtains the relation between the Eulerian angles of the texture component and peaks in two 'unreduced' PF (Bukharova, 1990). For example, the angle β_0 is given by

$$\beta_0 = \arccos\left\{\frac{1}{|[\mathbf{h}_1,\ \mathbf{h}_2]|^2} \{[\mathbf{y}_1,\ \mathbf{y}_2]^3[\mathbf{h}_1,\ \mathbf{h}_2]^3 + y_1^3\ (h_1^3 - h_2^3\ (\mathbf{h}_1,\ \mathbf{h}_2)) + \\ + \mathbf{y}_2^3\ (h_2^3 - h_1^3\ (\mathbf{h}_1,\ \mathbf{h}_2))\}\right\}. \tag{7}$$

DETERMINATION OF THE ORIENTATION OF ISOLATED TEXTURE COMPONENTS FROM POLE FIGURES IN THE CASE OF TRICLINIC CRYSTAL SYMMETRY

Now we assume that the pole figures would be obtained by 'normal' diffraction experiments. For PF $\tilde{P}_{\mathbf{h}}(\mathrm{y})$ obtained by 'normal' diffraction experiments and 'unreduced' PF $P_{\mathbf{h}}(\mathbf{y})$ the relation

$$\tilde{P}_{\mathbf{h}}(\mathrm{y}) = [P_{\mathbf{h}}(\mathbf{y}) + P_{-\mathbf{h}}(\mathbf{y})]/2 \tag{8}$$

is valid. In the case of triclinic crystal symmetry (point groups C_1, C_i) a peak at g_0 in the orientation space provides two peaks in the PF $\tilde{P}_{\mathbf{h}i}$ $(\mathbf{y})$ at $\pm\mathbf{y}_i$, where $\mathbf{y}_i = T(g_0)\mathbf{h}'_i$. As a result instead of the system of Eq. (2) we get four different systems

$$(a)\begin{cases} \mathbf{y}'_1 = T(g_0)\mathbf{h}'_1 \\ \mathbf{y}'_2 = T(g_0)\mathbf{h}'_2 \end{cases} (b)\begin{cases} -\mathbf{y}'_1 = T(g_0)\mathbf{h}'_1 \\ \mathbf{y}'_2 = T(g_0)\mathbf{h}'_2 \end{cases} (c)\begin{cases} \mathbf{y}'_1 = T(g_0)\mathbf{h}'_1 \\ -\mathbf{y}'_2 = T(g_0)\mathbf{h}'_2 \end{cases} (d)\begin{cases} -\mathbf{y}'_1 = T(g_0)\mathbf{h}'_1 \\ -\mathbf{y}'_2 = T(g_0)\mathbf{h}'_2 \end{cases}. \tag{9}$$

The solutions of these systems are given by Eq. (5) with (*a*), $\mathbf{h}_1$, $\mathbf{h}_2$, $\mathbf{y}_1$, $\mathbf{y}_2$, (*b*) $\mathbf{h}_1$, $\mathbf{h}_2$, $-\mathbf{y}_1$, $\mathbf{y}_2$, (c) $\mathbf{h}_1$, $\mathbf{h}_2$, $\mathbf{y}_1$, $-\mathbf{y}_2$, (*d*) $\mathbf{h}_1$, $\mathbf{h}_2$, $-\mathbf{y}_1$, $-\mathbf{y}_2$, respectively.

Statement 1. If $(\mathbf{h}_1, \mathbf{h}_2) \neq 0$ then only in two cases of (*a*) - (*d*) the solution of the system is an orientation matrix.

The statement is proved easily by going over from the crystal coordinate system K_B to crystal coordinate system $\tilde{K}_B$ in which the coordinates of the vectors $\mathbf{h}_1$ and $\mathbf{h}_2$ are equal to

$$\tilde{\mathbf{h}}_1 = (1, 0, 0), \quad \tilde{\mathbf{h}}_1 = (\cos\varphi, \sin\varphi, 0). \tag{10}$$

Let us denote the rotation which transforms K_A into $\tilde{K}_B$ by $\tilde{g}_0$. The connections between g_0 and $\tilde{g}_0$ and between $T(g_0)$ and $T(\tilde{g}_0)$ are given by (Bunge, 1982)

$$g_0 = \tilde{g}_B^{-1}\tilde{g}_0, \quad T(g_0) = T^{-1}(\tilde{g}_B)T(\tilde{g}_0)T(\tilde{g}_B), \tag{11}$$

where $\tilde{g}_B$ is the rotation which transforms $\tilde{K}_B$ into K_B. It can be straightforward verified that only in two cases of (*a*) – (*d*) the solution of the system is an orthogonal matrix with determinant equal to 1. These matrices yield two orientations, namely, the correct orientation $\tilde{g}_0^c \equiv \tilde{g}_0 = \{\tilde{\alpha}_0, \tilde{\beta}_0, \tilde{\gamma}_0\}$ and an uncorrect orientation $\tilde{g}_0^u$, which is expressed in terms of correct orientation as follows

$$\tilde{g}_0^u = \hat{2}_z\tilde{g}_0^c = \{\tilde{\alpha}_0, \tilde{\beta}_0, \tilde{\gamma}_0 + \pi\}, \tag{12}$$

where $\hat{2}_z$ is a rotation is the second order around the axis $Z_{\tilde{B}}$.

It should be mentioned the situation when the vectors $\mathbf{h}_1$ and $\mathbf{h}_2$ are perpendicular to each other. As it can be shown in this case two PF yield four orientations which are related to each other by the elements of the rotation group D_2

$$\begin{aligned} \tilde{g}_0^1 &= \tilde{g}_0^c = \{\tilde{\alpha}_0, \tilde{\beta}_0, \tilde{\gamma}_0\}, & \tilde{g}_0^2 &= \hat{2}_x\tilde{g}_0^c = \{\pi + \tilde{\alpha}_0, \pi - \tilde{\beta}_0, 2\pi - \tilde{\gamma}_0\}, \\ \tilde{g}_0^3 &= \hat{2}_y\tilde{g}_0^c = \{\pi + \tilde{\alpha}_0, \pi - \tilde{\beta}_0, \pi - \tilde{\gamma}_0\}, & \tilde{g}_0^4 &= \hat{2}_z\tilde{g}_0^c = \{\tilde{\alpha}_0, \tilde{\beta}_0, \pi + \tilde{\gamma}_0\}. \end{aligned} \tag{13}$$

Now let us consider three PF $\tilde{P}_{\mathbf{h}_1}(\mathbf{y})$, $\tilde{P}_{\mathbf{h}_2}(\mathbf{y})$, $\tilde{P}_{\mathbf{h}_3}(\mathbf{y})$.

Statement 2. If $(\mathbf{h}_1, [\mathbf{h}_2, \mathbf{h}_3]) \neq 0$ and each of the vectors $\mathbf{h}_1$, $\mathbf{h}_2$, $\mathbf{h}_3$ is not parallel to the vector product of the remaining ones, then the correct solution $g_0 = \{\alpha_0, \beta_0, \gamma_0\}$ can be obtained.

The statement is based on the result that only one solution is preset simultaneously in both sets of solutions (Bukharova, 1990). The Correct orientation is defined as the intersection of these sets of solutions

$$g_0 = \left\{ \begin{array}{c} \textit{orientations obtained} \\ \textit{from } \tilde{P}_{\mathbf{h}_1}(\mathbf{y}),\ \tilde{P}_{\mathbf{h}_2}(\mathbf{y}) \end{array} \right\} \bigcap \left\{ \begin{array}{c} \textit{orientations obtained} \\ \textit{from } \tilde{P}_{\mathbf{h}_1}(\mathbf{y}),\ \tilde{P}_{\mathbf{h}_3}(\mathbf{y}) \end{array} \right\}. \tag{14}$$

At last, we have to consider the case when the texture consists of few non-overlapping components, reflected to non-overlapping components in the pole figures $\tilde{P}_{\mathbf{h}_1}(\mathbf{y})$, $\tilde{P}_{\mathbf{h}_2}(\mathbf{y})$, $\tilde{P}_{\mathbf{h}_3}(\mathbf{y})$, too. N peaks in the orientation space provide $2N$ peaks in the pole figure $\tilde{P}_{\mathbf{h}_i}(\mathbf{y})$ at $\pm\mathbf{y}_i^1, \pm\mathbf{y}_i^2, ..., \pm\mathbf{y}_i^N$, $i = 1, 2, 3$. The set of vectors $\{\pm\mathbf{y}_1^1, ..., \pm\mathbf{y}_1^N, \pm\mathbf{y}_2^1, ..., \pm\mathbf{y}_2^N, \pm\mathbf{y}_3^1,$

$\pm\mathbf{y}_3^N\}$ has to be split up into N sets $\{\pm\mathbf{y}_1^i, \pm\mathbf{y}_2^j, ..., \pm\mathbf{y}_3^k\}$, $i = 1, 2, ..., 3$, by using the conditions

$$(\mathbf{y}_1^i, \mathbf{y}_2^j) = \pm(\mathbf{h}_1^i, \mathbf{h}_2^j), \quad (\mathbf{y}_1^i, \mathbf{y}_3^k) = \pm(\mathbf{h}_1^i, \mathbf{h}_3^k), \quad (\mathbf{y}_2^j, \mathbf{y}_3^k) = \pm(\mathbf{h}_2^j, \mathbf{h}_3^k). \tag{15}$$

The orientation g_0^i, $i = 1, 2, ..., N$, is determined unambiguously by the set $\{\pm\mathbf{y}_1^i, \pm\mathbf{y}_2^j, \pm\mathbf{y}_3^k\}$ with the help of Eq. (5), (14).

INFLUENCE OF MONOCLINIC CRYSTAL SYMMETRY ON THE DETERMINATION OF THE ORIENTATION OF ISOLATED TEXTURE COMPONENTS FROM POLE FIGURES

Monoclinic crystal system contains three crystal classes: $C_2 = \{\hat{2}_z\}$, $C_3 = \{m\}$, $C_{2h} = \{\hat{2}_z, m\}$. Let g_0 be a peak in the orientation space. The rotational part of the groups C_2, C_{2h} is the group C_2. Hence, two equivalent peaks at g_0 and at $\hat{2}_z g_0$ exist in the orientation space. The rotational part of the group C_3 is the group C_1. Hence, a single peak at g_0 exists in the orientation space. Because the groups C_2, C_3 and C_{2h} give rise to the common Laue group C_{2h}, the PF are identical for all these groups. The orientation g_0 can be reproduced from PF within the multiplication from the left to the element $\hat{2}_z$ of the rotation group C_2. For the groups C_2 and C_{2h} both g_0 and $\hat{2}_z g_0$ are solutions of the problem. For the group C_3 this is not the case. Consequently, in the case of the group C_3 the orientation of an isolated texture component is not determined unambiguously from PF.

For the groups C_2 and C_{2h} the orientation of an isolated texture component can be determined from two PF $\tilde{P}_{\mathbf{h}_1}$ and $\tilde{P}_{\mathbf{h}_1}$ with $\mathbf{h}_1 = (1, 0, 0)$ and $\mathbf{h}_2 = (\cos\varphi, \sin\varphi, 0)$. This statement is based on the fact that peaks at g_0 and at $\hat{2}_z g_0$ in the orientation space provide two peaks in any of these PF. Consequently, Eq. (12) is valid. It gives the solution of the problem.

CONCLUSION

With the help of the explicit relationship between the orientation of isolated texture components and peaks in pole figures the influence of crystal symmetry on the determination of this orientation from different PF can be considered. In the special case that the problem is not ill-posed the number of PF sufficient to determine the orientation of isolated texture components unambiguously depends on crystal symmetry and on the symmetry of measured PF. In the case of triclinic crystal symmetry three PF $\tilde{P}_{\mathbf{h}_1}(\mathbf{y})$, $\tilde{P}_{\mathbf{h}_2}(\mathbf{y})$, $\tilde{P}_{\mathbf{h}_3}(\mathbf{y})$ provide an unambiguous result on the condition that $((\mathbf{h}_1, [\mathbf{h}_2, \mathbf{h}_3]) \neq 0)$ and each of the vectors $\mathbf{h}_1$, $\mathbf{h}_2$, $\mathbf{h}_3$ is not parallel to the vector product of remaining ones. In the case of monoclinic crystal symmetry (point groups C_2, C_{2h}) the orientation of an isolated texture component is determined unambiguously from two PF $\tilde{P}_{\mathbf{h}_1}(\mathbf{y})$, $\tilde{P}_{\mathbf{h}_2}(\mathbf{y})$ with $\mathbf{h}_1 = (h_1^1, h_1^2, 0)$, $\mathbf{h}_2 = (h_2^1, h_2^2, 0)$. For the group C_3 it is not determined unambiguously from PF.

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