APPLICATION OF NORMAL DISTRIBUTIONS ON $SO(3)$ AND S^n FOR ORIENTATION DISTRIBUTION FUNCTION APPROXIMATION

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The orientation distribution function (ODF) in a polycrystalline sample is of special interest in texture analysis. Its determination from pole figures leads to an ill-posed problem, the solution of which is non-unique.

In the present paper the properties of normal distributions on the rotation group $SO(3)$ proposed by Parthasarathy (1964), Savyolova (1984) are discussed. A method for ODF determination based on the superposition of the normal distributions is proposed. The parameters of normal distributions are determined from the experimental pole figures. The application of this method is demonstrated for a rolling texture of beryllium.

KEY WORDS Normal distributions, ODF approximation, hexagonal symmetry, rolling texture of beryllium

INTRODUCTION

The central problem of the quantitative texture analysis is the determination of the orientation distribution function of texturized samples from pole figures measured by X-ray or neutron diffraction techniques. The most widely applied method to solve this problem is the series expansion formalism proposed by Bunge (1969). It is not capable of avoiding regions of negative values and ghost effects in the ODF. The reason for these phenomena was revealed by Matthies (1979). He showed that ghost effects are caused by the lack of information on the odd part of the ODF and, consequently, it is in principle not possible to determine the "true" ODF from pole figure data. This discovery stimulated the development of numerous approaches for the ODF determination from pole figures by using additional information on ODF. One such approach consists in using special model functions. Pospiech (Cracow) and Lucke (Aachen) groups got valuable results in ODF representation by a finite number N of normalized bell-shaped distributions on $SO(3)$. In their papers (1981, 1986) the authors have used a Gaussian type function suggested by Bunge (1969) for the bell-shaped distribution. However, this function possesses several disadvantages. One of them is that it cannot adequately describe the whole width of the spectrum for bell-shaped curves beginning with very sharp peaks up to the random distribution. Moreover, there is no explicit analytical expression for the corresponding pole figures, and therefore the "Gaussian" component fit cannot be directly

achieved from the pole figures. A new method for ODF determination from experimental pole figures was proposed in (Nicolae, Savyolova, Feldmann, 1992). In this method, the ODF is represented by a superposition of a number of normal distributions, suggested by Savyolova (1984). Basing on the known analytical relationships between ODF's and pole figures formed by such type of distributions, the parameters of normal distributions are found from experimental data for cubic lattice symmetry.

In the present paper we take the normal distribution on the rotation group which satisfies the central limit theorem in Parthasarathy K. P. (1964). The properties of these normal distributions are discussed. It is possible to obtain explicit expressions for the density of normal distribution only for specific cases. One of such cases is the central normal distribution. The connection of the central normal distribution on SO(3) group with fundamental solution of the corresponding diffusion equation is shown (see Perrin, 1928, Roberts, Winch, 1984, Heyer, 1987). Some projections of the normal distribution are obtained. These projections coincide with the normal distribution on the unit circle (Mardia, 1972) and with the Perrin distribution on the two dimensional unit sphere (Perrin, 1928).

In the paper (Matthies, Muller and Vinel, 1988) the central normal distribution are only analysed.

The analogues of the normal distribution for rotation group SO(3) and for hyperspheres S^n are discussed in (Schaefer, 1992, see also the references in this article).

In the present paper the central normal distributions are used for approximation of ODF. The calculations are illustrated for hexagonal lattice symmetry. The application of the proposed method is demonstrated for the example of the rolling texture of beryllium.

The canonical normal distributions are used for approximation of ODF in (Savyolova, 1989).

1. DEFINITIONS OF NORMAL DISTRIBUTION ON SO(3) AND S^2

1.1. The Term "normal distribution"

Normal distributions are widely used in practice in texture analysis (Bunge, 1969; Nikolaev, Savyolova, Feldmann, 1992; Savyolova, 1984; Matthies, Miller and Vinel, 1988). The first model of a central normal type distribution was proposed by Bunge

$$f(\varepsilon, \Phi) = N(\varepsilon) \exp [-(\Phi/\varepsilon)^2] \quad (1)$$

with

$$N(\varepsilon) = (2\pi)^{-1/2} [1 - \exp(-(\varepsilon/2)^2)],$$

$$\cos \Phi = (\text{Tr}(g_0^{-1}g) - 1)/2, \quad g_0, g \in \text{SO}(3).$$

Bunge's normal distribution (1) is an analogue of the normal distribution

$$f(x) = (2\pi)^{-1/2} \exp [-(x - x_0)^2/2\sigma^2]/\sigma,$$

investigated by Moivre, Laplace and Gauss and widely used in statistics. The normal distribution is important because it plays a special role due to its

characterization by the central limit theorem of probability theory. This theorem considers the function of the probability distribution of a quantity describing a sum of a large number of independent quantities all possessing their own probability distributions.

The rotation group $SO(3)$ has a complete set of irreducible representations $g \rightarrow T_g^{(1)}, g \rightarrow T_g^{(2)}, \dots$. Then $T_g^{(1)}, T_g^{(2)}, \dots$, may be considered as matrix functions on $SO(3)$ satisfying condition

$$T_{g_1}^{(n)} T_{g_2}^{(n)} = T_{g_1 g_2}^{(n)}, \quad n = 1, 2, \dots$$

We define the infinitesimal operators of a representation $g \rightarrow T_g$ as

$$A^i = \lim_{t \rightarrow 0} (T_{g_i(t)} - E)/t, \quad i = 1, 2, 3, \quad (2)$$

where E is the unit matrix of the same order as T_g , $g_i(t)$ are the parameters of group whose tangent vectors at unity are mutually orthogonal.

A distribution μ on a group G is said to be infinitely divisible if for every integer n exists a distribution μ_n such that $\mu = \mu_n^{*n}$, where $*$ denotes convolution.

A distribution μ on a group G is said to be an idempotent factor if $\mu^{*2} = \mu$.

DEFINITION 1 A distribution μ is said to be normal if it is infinitely divisible without idempotent factors and admits representation of the type

$$\int_{SO(3)} T_g d\mu(g) = \exp \left\{ \sum_{i,j=1}^3 \alpha_{ij} A^i A^j + \sum_{i=1}^3 \alpha_i A^i \right\}, \quad (3)$$

where A^i , $i = 1, 2, 3$ are the matrices (2), (α_{ij}) is a real positive definite or semidefinite matrix, and α_i , $i = 1, 2, 3$, are constants.

The central limit theorem for the rotation group $SO(3)$ gives the necessary and sufficient conditions under which the limit of a sequence of distributions of the type μ_n^{*n} may be normal (Parthasarathy, 1964; Savvolutova, 1984).

THEOREM If $n(1 - \det(g_n)) < C$, $C = \text{constant}$, $\lim_{n \rightarrow \infty} n(e - g_n) = \Gamma = (\gamma_{ij})$, then the limit of μ_n^{*n} exists and is a normal distribution whose parameters are given by

$$\begin{aligned} \alpha_i &= (\gamma_{jk} - \gamma_{kj})/2, \quad i \neq j \neq k, \quad j > i, \quad i, j, k = 1, 2, 3; \\ \alpha_{ii} &= (\gamma_{ii} - \gamma_{jj} - \gamma_{kk})/2, \quad i \neq j \neq k; \\ \alpha_{ij} &= \alpha_{ji} = -(\gamma_{ij} + \gamma_{ji})/2, \end{aligned}$$

where $g_n = \int_{SO(3)} g d\mu_n(g)$, e is the unit in $SO(3)$.

1.2. The Properties of Normal Distribution on $SO(3)$

The normal distribution $\mu(g)$, $g \in SO(3)$, (3) may be represented by a series expansion

$$f(g) = \sum_{l=0}^{\infty} \sum_{m,n=-l}^l C_l^{mn} T_l^{mn}(g), \quad (4)$$

where C_l^{mn} are the corresponding Fourier-type coefficients, $T_l^{mn}(g)$ are spherical functions on the group $SO(3)$. Let the three Eulerian angles $g = \{\alpha, \beta, \gamma\}$, $0 \leq \alpha, \gamma < 2\pi$, $0 \leq \beta \leq \pi$, be the three rotations with the help of these the coordinate

system K_A can be oriented parallel to K_B with $dg = \sin \beta d\alpha d\beta d\gamma$, where K_B is the coordinate system of a given crystal, and K_A is the coordinate system of the sample. In the present paper everywhere except for part 2.3 the choice of the Eulerian angles is the same as defined by Bunge (1969) $g = \{\alpha, \beta, \gamma\} = \{\varphi_1, \Phi, \varphi_2\}$. Putting the parameters $\alpha_i = 0$, $\alpha_{ij} = 0$, $i \neq j$, $i, j = 1, 2, 3$, into the relation (3) we obtain

$$\int_{\text{SO}(3)} T_g^l \sum_{l=0}^{\infty} \sum_{m,n=-l}^l C_l^{mn} T_l^{mn}(g) dg = \exp B_l \quad (l=0, 1, 2, \dots) \quad (5)$$

with $B_l = \sum_{i=1}^3 \alpha_{ii} (A_i^l)^2 = (b_{ij})$,

$$b_{1+m,1+m} = b_{2l+1-m,2l+1-m} = -[(2m+1)l - m^2](\alpha_{11} + \alpha_{22})/2 - (l-m)^2 \alpha_{33},$$

$$\begin{aligned} b_{1+m,3+m} &= b_{3+m,1+m} = b_{2l+1-m,2l-1-m} = b_{2l-1-m,2l+1-m} \\ &= -[(m+1)(m+2)(2l-m)(2l-1-m)]^{1/2}(\alpha_{11} - \alpha_{22})/4, \\ m &= 0, 1, \dots, l, \end{aligned}$$

the rest $b_{ij} = 0$.

For the unitary matrix B_l we obtain

$$B_l = (D_l)^{-1} \Lambda_l D_l,$$

where D_l is an orthogonal matrix, Λ_l is a diagonal matrix. Thus, we have

$$\exp B_l = (D_l)^{-1} \exp \Lambda_l D_l.$$

If $\alpha_{11} = \alpha_{22} = a^2$ in Eq. (5), we obtain

$$\begin{aligned} f(g) &= \sum_{l=0}^{\infty} (2l+1) \exp \{-l(l+1)a^2\} \sum_{m=-l}^l \exp \{m(a^2 - b^2) \\ &\quad - im(\alpha + \beta)\} P_l^{mn}(\cos \beta), \end{aligned} \quad (6)$$

Figure 1 The central normal distributions on the $\text{SO}(3)$ with the parameters $\varepsilon_k^2 = 2^{-k}$, $k = 0, 1, 2, 3$.

Figure 2 The normal distributions with the parameters 1—{1, 0, 1}, 2—{1, 1, 0}, 3—{0, 1, 1}, 4—{1, 1, 1} where $\alpha = 0^\circ$, $\beta = 10^\circ$.

Figure 3 The normal distributions with the same parameters as in Figure 2 where $\gamma = 0^\circ$, $\beta = 10^\circ$.

where $P_l^{mn}(\cos \beta)$ are Jacobi polynomials (Vilenkin, 1965). Let $a^2 = b^2 = \varepsilon^2$ in (6). Then we obtain the central normal distribution

$$f(g) = f_1(t) = \sum_{l=0}^{\infty} (2l+1) \exp \{ -l(l+1)\varepsilon^2 \} \sin((l+1/2)t) / \sin(t/2), \quad (7)$$

where $\cos(t/2) = \cos(\beta/2) \cos((\alpha + \gamma)/2)$ (Vilenkin, 1965).

If $\alpha_i = 0$, $\alpha_{ij} = 0$, $i, j = 1, 2, 3$, except $\alpha_{33} = b^2 > 0$, we obtain the normal distribution on the circle $SO(2)$ (Mardia, 1972)

$$f(g) = f_2(\beta) = (2\pi)^{-1/2} \sum_{l=0}^{\infty} \exp \{ -(\beta + 2\pi l)^2 / 2\sigma^2 \} / \sigma, \quad \sigma = b(2)^{1/2}. \quad (8)$$

In Figure 1 the central normal distributions (7) are shown with the parameters $\varepsilon_k^2 = 2^{-k}$, $k = 0, 1, 2, 3$. In Figure 2 the normal distributions (5) are displayed with the parameters $\{\alpha_{11}, \alpha_{22}, \alpha_{33}\}$: 1—{1, 0, 1}, 2—{1, 1, 0}, 3—{0, 1, 1}, 4—{1, 1, 1}, where $\alpha = 0^\circ$, $\beta = 10^\circ$. In Figure 3 the normal distributions (5) are shown with the same parameters as in Figure 2, where $\gamma = 0^\circ$, $\beta = 10^\circ$.

1.3. Normal Distribution on Sphere S^2

The set of classes $\{uh\}$ can be identified with the sphere S^2 in R^3 (Vilenkin, 1965), where $u \in SU(2)$ is the element of the unitary unimodular group, $h \in \Omega$ is the subgroup with the elements

$$h = \begin{pmatrix} \exp(it/2) & 0 \\ 0 & \exp(it/2) \end{pmatrix}.$$

The function $f(\xi)$, $\xi \in S^2$ can be obtained from function $f(u)$, $u \in SU(2)$, for which we have $f(uh) = f(u)$. The infinitesimal operator A^3 corresponds to the subgroup Ω . Hence, we can define the normal distribution on the sphere S^2 from normal distribution on the group $SO(3)$ (3) if we put $\alpha_3 = 0$, α_{3j} and $\alpha_{j3} = 0$, $j = 1, 2, 3$.

DEFINITION 2 A normal distribution $f(\xi)$, $\xi \in S^2$ on the sphere S^2 can be obtained from the normal distribution on the group $SO(3)$ (3), where $\alpha_3 = 0$,

Figure 4 The central normal distributions on the S^2 with the parameter $\alpha_k^2 = 2^{-k}$, $k = 0, 1, 2, 3$.

$\alpha_{3j} = 0$ and $\alpha_{j3} = 0$, $j = 1, 2, 3$:

$$\begin{aligned} f(\xi) d\xi &= (8\pi^2)^{-1} \int_0^{2\pi} (f(g) \sin \beta d\alpha d\beta) d\gamma \\ &= (4\pi)^{-1} \sum_{l=0}^{\infty} \sum_{m=-l}^l C_l^{m0} T_l^{m0}(g) \sin \beta d\beta d\alpha. \end{aligned}$$

If the parameters $\alpha_{11} = \alpha_{22} = a^2$, $\alpha_{12} = \alpha_{21} = 0$, we get

$$f(\beta) = \sum_{l=0}^{\infty} (2l+1) \exp \{-l(l+1)a^2\} P_l(\cos \beta), \quad (9)$$

where $P_l(\cos \beta)$ are Legendre polynomials.

In Figure 4 the normal distributions (9) are shown for the parameters $a_k^2 = 2^{-k}$, $k = 0, 1, 2, 3$.

The central normal distribution (9) has been obtained by Perrin (1928) for the Brownian motion on the sphere S^2 in the space R^3 . In Appendix A we give the definition of normal distribution on the sphere S^{n-1} in the space R^n , $n > 2$, as a solution of the parabolique differential equation.

2. APPLICATION OF CENTRAL NORMAL DISTRIBUTIONS FOR ODF APPROXIMATION FOR HEXAGONAL LATTICE SYMMETRY

2.1. Formulation of Problem

The orientation distribution of grains in polycrystalline samples is described by an ODF $f(g)$, where g belongs to the rotation group $SO(3)$ with

$$\int_{SO(3)} f(g) dg = 8\pi^2.$$

X-ray and neutron methods of texture investigation are used to get the experimental pole figures (PF) $\tilde{P}_{\vec{h}}(\vec{y})$, $i = 1, 2, \dots, l$. The PF $\tilde{P}_{\vec{h}}(\vec{y})$ is defined by the integral of the ODF $f(g)$ over all those orientations for which the crystal direction $\pm\vec{h}$ is parallel to the sample direction $\vec{y}$ (Bunge, 1969)

$$\tilde{P}_{\vec{h}}(\vec{y}) = (4\pi)^{-1} \int_{[\pm\vec{h}||\vec{y}]} f(g) d\psi, \quad (10)$$

with

$$\int_{\vec{y} \in S^2} \tilde{P}_{\vec{h}}(\vec{y}) d\vec{y} = 4\pi.$$

The problem of getting ODF $f(g)$ from experimental pole figures is an ill-posed problem, the solution of which is nonunique (Matthies, 1979). Additional information—for example, additional model type suppositions—is necessary. In the present paper it is assumed that the true texture function is a superposition of the central normal distributions (7).

If the centre of the central normal distribution is $g_0 \neq \{0, 0, 0\}$, $g_0 \in \text{SO}(3)$, then the formula

$$f(g, g_0, \varepsilon) = f_1(t), \quad (11)$$

where $\cos t = [\text{Tr}(g_0 g^{-1}) - 1]/2$, has to be used instead of the (7). The corresponding PF has the form

$$\tilde{P}_{\vec{h}}(\vec{y}, g_0, \varepsilon) = P_1(\theta) = \sum_{l=0}^{\infty} (4l+1) \exp\{-2l(2l+1)\varepsilon^2\} P_{2l}(\cos \theta), \quad (12)$$

where $\cos \theta = (\vec{h}, g_0 \vec{y})$ is the scalar product of $\vec{h}$ and $g_0 \vec{y}$. The derivation of the formula (12) is given in the Appendix B.

We get the formulas

$$f_1(t) = \left[\frac{\pi}{\varepsilon^3} \exp(\varepsilon^2/4) \text{erfc}(\varepsilon/2) + 1/\varepsilon^2 \right] \frac{t/2}{\sin(t/2)} \exp(-t^2/4\varepsilon^2), \quad (13)$$

if $\varepsilon < 0.5$, and

$$\tilde{P}_1(\theta) \approx \frac{1}{2\varepsilon^2} [\exp(-\theta^2/4\varepsilon^2) + \exp(-(\pi - \theta)^2/4\varepsilon^2)], \quad (14)$$

if $\varepsilon < 0.3$, in place of the formulas (11) and (12) respectively.

If a crystal or sample symmetry is present it can be taken into account by using the following averaging rule

$$f^s(g, g_0, \varepsilon) = \frac{1}{N_A N_B} \sum_{i=1}^{N_A} \sum_{j=1}^{N_B} f(g, g_{Bj} g_0 g_{Ai}, \varepsilon), \quad (15)$$

$$\tilde{P}_{\vec{h}}^s(\vec{y}, g_0, \varepsilon) = \frac{1}{M_A M_B} \sum_{i=1}^{M_A} \sum_{j=1}^{M_B} \tilde{P}_{r_{Bj}\vec{h}}(r_{Ai}\vec{y}, g_0, \varepsilon), \quad (16)$$

where $R_A = \{r_{Ai}, i = 1, 2, \dots, M_A\}$, $R_B = \{r_{Bi}, i = 1, 2, \dots, M_B\}$ are the groups of specimen symmetry and crystal symmetry respectively, $G_A = \{g_{Ai}, i = 1, 2, \dots, N_A\}$, $G_B = \{g_{Bi}, i = 1, 2, \dots, N_B\}$ are their rotation subgroups. The axial texture for central normal distribution with axis $\vec{n}_t$ may be found from

formulas (11) and (12) by integration (Bucharova *et al.*, 1988):

$$f^A(g, g_0, \varepsilon, \vec{n}_t) = \sum_{l=0}^{\infty} (2l+1) \exp \{-l(l+1)\varepsilon^2\} P_l(\cos \tilde{\beta}), \quad (17)$$

$$\tilde{P}_h^A(y, g_0, \varepsilon, \vec{n}_t) = \sum_{l=0}^{\infty} (4l+1) \exp \{-2l(2l+1)\varepsilon^2\} P_{2l}(\cos \theta_1) P_{2l}(\cos \theta_2), \quad (18)$$

where $\cos \tilde{\beta} = (g\vec{n}_t, g_0\vec{n}_t)$, $\cos \theta_1 = (\vec{h}, g_0\vec{n}_t)$, $\cos \theta_2 = (\vec{y}, \vec{n}_t)$.

We consider polycrystalline samples for hexagonal lattice symmetry with crystal symmetry D_{6h} and with orthorhombic specimen symmetry. Then the coefficients in Eq. (15) with $l = 1, 3, 5$ are equal to zero. When ε is large enough (weak texture), the function $f^s(g, g_0, \varepsilon)$ and the sum of its terms with even numbers $l \sqcup \tilde{f}^s(g, g_0, \varepsilon)$ are almost equal if $\varepsilon > 0.3$. If $\varepsilon < 0.3$ (sharp texture) the functions $f^s(g, g_0, \varepsilon)$ and $\tilde{f}^s(g, g_0, \varepsilon)$ are different ($\tilde{f}^s$ has negative values and ghost effects). Then for ODF determination from experimental data we approximate the ODF by normal distributions.

Consider the next method of solving the problem for ODF determination from experimental pole figures.

Let ODF $f(g)$ be a superposition of central normal distributions

$$f(g) = \sum_{n=1}^N M_n f^s(g, g_n, \varepsilon_n), \quad \sum_{n=1}^N M_n = 1, \quad (19)$$

where N is the number of components of texture, M_n is the weight of n -th component, g_n is the coordinate of the centre, ε_n is the width. Taking Eq. (19) into account, the pole figures may be written as

$$\tilde{P}_h^{\text{theor}}(\vec{y}) = \sum_{n=1}^N M_n \tilde{P}_h^s(\vec{y}, g_n, \varepsilon_n). \quad (20)$$

Now we must find the parameters of normal distributions. These parameters can be found using the method of minimization of the functional

$$\Phi = \sum_{i=1}^I \int_{\vec{y} \in S^2} (\tilde{P}_{h_i}^{\text{exp}}(\vec{y}) - \tilde{P}_{h_i}^{\text{theor}}(\vec{y}))^2 d\vec{y} \rightarrow \min, \quad (21)$$

where $\tilde{P}_{h_i}^{\text{exp}}(\vec{y})$, $i = 1, 2, \dots, I$, are experimental pole figures.

2.2. Method of Calculation of ODF for Polycrystalline Sample of Hexagonal Lattice Symmetry

Consider the two steps of solving the problem (21):

Step 1. Determination of the number of components N of texture and their coordinates g_n .

Step 2. Determination of the parameters ε_n , M_n , $i = 1, 2, \dots, N$.

In case of hexagonal lattice symmetry with crystal symmetry D_{6h} the texture components can be distinguished if the positions of the maxima in the pole figures do not coincide (Bucharova and Savyolova, 1989). Then we can find the coordinates of the centres of normal distributions by the method described elsewhere (Bucharova and Savyolova, 1985).

If we know the coordinates of the centres of the normal distributions, then we can find the remaining parameters from Eq. (21) using the least squares method of minimization of the functional. We have a system of linear algebraic equations

$$A_l \vec{X}_l = \vec{B}_l, \quad l = 2, 4, 6, \dots, \quad (22)$$

where

$$\begin{aligned} a_l^{ij} &= \frac{1}{M_A N_B} \sum_{k=1}^l \sum_{n,n'=1}^{M_A} \sum_{m,m'=1}^{N_B} P_l((r_{An} g_j^{-1} g_{Bm} \vec{h}_k, r_{An'} g_i^{-1} g_{Bm'} \vec{h}_k)), \\ b_l^j &= \frac{1}{4\pi} \sum_{k=1}^l \int_{\vec{y} \in S^2} \bar{P}_{\vec{h}_k}^{\text{exp}}(\vec{y}) \sum_{n=1}^{M_A} \sum_{m=1}^{N_B} P_l((r_{An} g_j^{-1} g_{Bm} \vec{h}_k, \vec{y})) d\vec{y}, \\ x_l^j &= M_j \exp \{-l(l+1)\varepsilon_j^2\}, \quad i, j = 1, 2, \dots, N. \end{aligned}$$

Using the solution of system (22) with $l = l_1$ and l_2 , when the determinant of the system is not equal to zero, we get

$$\begin{aligned} \varepsilon_i^2 &= \ln(x_{l_1}^i / x_{l_2}^i) / [l_2(l_2 + 1) - l_1(l_1 + 1)], \\ M_i &= x_{l_1}^i \exp \{l_1(l_1 + 1)\varepsilon_i^2\}. \end{aligned}$$

The influence of certain experimental errors in pole figure determination—namely, the statistical fluctuations and the partitions of the pole sphere—on the stability of this algorithm has been studied by computer simulation. The results of model calculations show that this algorithm is stable for texture with isolated components.

If the positions of components of texture are not isolated, additional conditions, such as the minimum number of normal distributions, or other considerations, have to be taken into account.

2.3. Numerical Results

An application of the proposed method is demonstrated by the example of a rolling texture of beryllium produced by rolling of the fiber texture with axis $\vec{n}_i = \{0^\circ, 0^\circ\}$, $g_0 = \{\alpha, 90^\circ, 0^\circ\}$, $\alpha \in [0^\circ, 360^\circ]$. In this example the sample coordinate system K_A and the crystal coordinate system K_B are fixed as follows: Z_A is parallel to the rolling direction (RD), X_A is parallel to the transverse direction (TD), and Y_A is parallel to the normal direction (ND); X_B , Y_B , Z_B are parallel to the crystal directions $[10\bar{1}0]$, $[\bar{1}2\bar{1}0]$ and $[0001]$ respectively. In this part of the paper the Eulerian angles are chosen as in (Roy, 1965) $g = \{\alpha, \beta, \gamma\} = \{\Psi, \Theta, \Phi\}$. The experimental PF $\{0001\}$, $\{10\bar{1}0\}$ and $\{10\bar{1}1\}$, obtained from X-ray measurements, are shown in Figures 5a, 6a, 7a respectively. For this texture it is difficult to find the number of components N and the coordinates of their centres from the positions of the maxima of function $\bar{P}_{\vec{h}}^{\text{exp}}(\vec{y})$ (Bucharova and Savyolova, 1989). We have used the method of minimization of the functional (21) with the two PF $\{0001\}$ and $\{10\bar{1}0\}$, taking into account the minimum number of normal distributions. Choosing different N ($N \geq 1$) and g_i , we find the parameters of ODF as a superposition of normal distributions

$$\begin{aligned} f(g) &= M_1 f_1(g, g_1, \varepsilon_1, \vec{n}_{i1}) + M_2 f_2(g, g_2, \varepsilon_2, \vec{n}_{i2}) + M_3 f_3(g, g_3, \varepsilon_3, \vec{n}_{i3}) \\ &\quad + M_4 f_4(g, g_4, \varepsilon_4, \vec{n}_{i4}) + M_5 f_5(g, g_5, \varepsilon_5, \vec{n}_{i5}) + M_6 f_6(g, g_6, \varepsilon_6) + M_7 f_7, \end{aligned}$$

Figure 5 Pole figure {0001}: a—experimental, b—calculated.

where f_1, f_2, f_3, f_4, f_5 are the axial components that can be given by Eq. (17) with parameters $\varepsilon_1 = 0.15$, $g_1 = \{90^\circ, 90^\circ, \gamma\}$, $\vec{n}_{t1} = \{90^\circ, 90^\circ\}$, $\varepsilon_2 = \varepsilon_3 = 0.125$, $g_2 = \{70^\circ, 90^\circ, \gamma\}$, $\vec{n}_{t2} = \{90^\circ, 70^\circ\}$, $g_3 = \{110^\circ, 90^\circ, \gamma\}$, $\vec{n}_{t3} = \{90^\circ, 110^\circ\}$, $\varepsilon_4 = \varepsilon_5 = 0.15$, $g_4 = \{50^\circ, 90^\circ, \gamma\}$, $\vec{n}_{t4} = \{90^\circ, 50^\circ\}$, $g_5 = \{130^\circ, 90^\circ, \gamma\}$, $\vec{n}_{t5} = \{90^\circ, 130^\circ\}$, $\gamma \in [0, 60^\circ]$. The component f_6 is the normal distribution of kind (15) with parameters $\varepsilon_6 = 0.15$, $g_6 = \{90^\circ, 90^\circ, 0^\circ\}$, and $f_7 \equiv 1$ is the isotropic distribution. The weights of components are: $M_1 = 0.37$, $M_2 = M_3 = 0.17$, $M_4 = M_5 = 0.06$, $M_6 = 0.08$, $M_7 = 0.09$.

The calculated PF {0001}, {10 $\bar{1}$ 0} and {10 $\bar{1}$ 1} are displayed in Figures 5b, 6b and 7b respectively.

The errors of even part of ODF of the proposed method can be estimated from the following relations (Roe, 1965; Matthies, 1986)

$$\sigma^2 = \int_{\vec{y} \in S^2} [P_{\vec{h}}^{\text{exp}}(\vec{y}) - P_{\vec{h}}^{\text{theor}}(\vec{y})]^2 d\vec{y},$$

$$RP(\Delta) = \frac{1}{J'} \sum_{j=1}^{J'} |P_{\vec{h}}^{\text{exp}}(\vec{y}_j) - P_{\vec{h}}^{\text{theor}}(\vec{y}_j)| \frac{100\%}{P_{\vec{h}}^{\text{exp}}(\vec{y}_j)},$$

where $P_{\vec{h}}^{\text{exp}}(\vec{y}_j) > \Delta > 0$. We get the following values of parameters σ and $RP(\Delta)$: PF {0001} — $\sigma = 0.42$, $RP(0.5) = 9\%$, $RP(1) = 6\%$; PF {10 $\bar{1}$ 0} — $\sigma = 0.48$, $RP(0.5) = 7\%$, $RP(1) = 6\%$; PF {10 $\bar{1}$ 1} — $\sigma = 0.42$, $RP(0.5) = 9\%$, $RP(1) = 7\%$.

Although the pole figure {10 $\bar{1}$ 1} is not used in this example, the comparison between the experimental data and the calculations for PF {10 $\bar{1}$ 1} yields the same error as for PF {0001} and {10 $\bar{1}$ 0}.

Figure 6 Pole figure {10 $\bar{1}$ 0}: a—experimental, b—calculated.

Figure 7 Pole figure $\{10\bar{1}1\}$: a—experimental, b—calculated.

Figures 8 and 9 shows sections of the ODF $f(g)$ and of its even part $\bar{f}(g)$ at constant γ . The degree of expansion of all ODF components, $l_{\max} = 30$, has been chosen so that the truncation error in the area of the ODF's maximum does not exceed 0.1%. For comparison, the ODF determined by the Roe–Bunge method using three experimental PF $\{0001\}$, $\{10\bar{1}0\}$ and $\{10\bar{1}1\}$ is displayed in Figure 10 ($l_{\max} = 16$). We see that the representation of the ODF as a superposition of normal distributions provides the following characteristics: the ODF satisfies the positivity condition and is free of ghost effects.

We use all information in pole figures for approximating the ODF by

Figure 8 ODF $f(g)$ of rolling texture of beryllium.

Figure 9 The even part of ODF $\bar{f}(g)$ (areas of negative values are hatched).

Figure 10 Representation of the ODF $f(g)$ by Roe-Bunge method (areas of negative values are hatched).

superposition of a number of normal distributions. Certainly, we can make a mistake if we define the odd part of ODF by the odd part of superposition of central normal distributions. The check of the odd part of the ODF can be made by other methods. We can find ODF as the sum of δ -functions on group SO(3) (Bucharova and Savyolova, 1985, 1989). Also, we can define the orientations of grains in polycrystalline sample (about 1000 grains) (Bunge, 1969), and then we must use a conventional χ^2 -test.

CONCLUSION

In the present paper normal distributions on SO(3) and S^n , $n \geq 2$, proposed by Parthasarathy (1964), Savyolova (1984) are discussed. The normal distributions on SO(3) satisfy the central limit theorem. The central normal distributions are used for approximating the ODF. The application of this method is illustrated with an example of the rolling texture of beryllium. The ODF approximated as a number of central normal distributions satisfies the positively condition and is free from ghost effects if the positions of maxima are isolated on pole figures. One or two poles figures are necessary for hexagonal lattices to determine the ODF by the proposed method, and three or more pole figures are necessary to determine the ODF by the Bunge-Roy method.

APPENDIX A

We consider the equation

$$\frac{1}{\sin^{n-2} \Theta} \frac{\partial}{\partial \Theta} \left(\sin^{n-2} \Theta \frac{\partial f}{\partial \Theta} \right) = \frac{1}{R} \frac{\partial f}{\partial t}, \quad (\text{A1})$$

where $f = f(\Theta, t)$, $\Theta \in [0, \pi]$, $R > 0$, $t > 0$. The solution of (A1) with $S_{n-1} \int_0^\pi f_{n-1}(\Theta, t) \sin^{n-2} \Theta d\Theta = 1$, $f_{n-1}(\Theta, 0) = \delta(\Theta)/S_{n-1}$, $S_{n-1} = 2\pi^{n/2}/\Gamma(n/2)$, $f_{n-1}(\theta, t) = F_{n-1}(u, t)$, $u = \cos \Theta$, is

$$f_{n-1}(\Theta, t) = F_{n-1}(u, t) = (2pS_{n-1})^{-1} \sum_{l=0}^{\infty} (2l+2p) \exp \{-l(l+2p)Rt\} C_l^p(u), \quad (\text{A2})$$

where $p = (n-2)/2 > 0$, $C_l^p(u)$ are the Ghegenbowar polynomials (Vilenkin, 1965). If $n = 2$, we have in (A2)

$$\begin{aligned} F_1(u, t) &= (2\pi)^{-1} \sum_{l=0}^{\infty} 2l \exp \{-l^2 Rt\} C_l^0(u) \\ &= \pi^{-1} \sum_{l=0}^{\infty} \exp \{-l^2 Rt\} \cos(l\Theta), \end{aligned}$$

the normal distribution on the circle SO(2) (8) which we get from definition (3). If $n = 3$ in (A2), we obtain

$$F_2(u, t) = (4\pi)^{-1} \sum_{l=0}^{\infty} (2l+1) \exp \{-l(l+1)Rt\} P_l(u), \quad (\text{A3})$$

the normal distribution on the sphere S^2 in the space R^3 (9). If $n = 4$, we have

$$F_3(u, t) = (4\pi^2)^{-1} \sum_{l=0}^{\infty} (2l+1) \exp \{-l(l+1)Rt\} \\ \times \sin((l+1)\Theta)/\sin \Theta, \quad \Theta \in [0, \pi], \quad (\text{A4})$$

the normal distribution on the sphere S^3 in R^4 or on the group $SU(2)$. If $l = 2m$, $m = 0, 1, \dots$ in (A4) we get

$$\tilde{F}_3(u, t) = (2\pi^2)^{-1} \sum_{l=0}^{\infty} (2l+1) \exp \{-l(l+1)4Rt\} \\ \times \sin((l+1/2)\tilde{\Theta})/\sin(\tilde{\Theta}/2), \quad \tilde{\Theta} = 2\theta,$$

the central normal distribution (7) on the group $SO(3)$.

APPENDIX B

The central normal distribution with the centre g_0 has the form

$$f(g, g_0, \varepsilon) = \sum_{l=0}^{\infty} F_l(\varepsilon) \sin((l+1/2)t)/\sin(t/2), \quad (\text{B1})$$

where $F_l(\varepsilon) = (2l+1) \exp \{-l(l+1)\varepsilon^2\}$, $g_0 = \{\alpha_0, \beta_0, \gamma_0\}$ and $\cos t = [\text{Tr}(g_0 g^{-1}) - 1]/2$ (Korn, G. and Korn, T., 1968).

Further, the following relation will be used

$$\frac{\sin((l+1/2)t)}{\sin(t/2)} = \sum_{m=-l}^l T_l^{mm}(g_0 g^{-1}) = \sum_{m,n=-l}^l T_l^{mn}(g_0) T_l^{nm}(g^{-1}), \quad (\text{B2})$$

where $T_l^{mn}(g) = \exp \{-i(m\alpha + n\gamma)\} P_l^{mn}(\cos \beta)$ (Vilenkin, 1965).

Let $\{\theta, \varphi\}$ and $\{\chi, \eta\}$ be the spherical angular coordinates of the crystal direction $\vec{h}$ in the crystal—fixed coordinate system K_B , and of the corresponding sample direction $\vec{y}$ in the sample—fixed system K_A , respectively. For the rotation g , which leads from K_A to K_B , it holds that

$$g = g_2 g_1,$$

where

$$g_1 = \left\{ \frac{\pi}{2} + \eta, \chi, 0 \right\}, \quad g_2 = \left\{ \frac{\pi}{2} + \varphi, \theta, \psi \right\}^{-1}, \quad \psi \in [0, 2\pi)$$

(Bunge, 1969). Now we fix the rotation g_1 , fix angles φ and θ of the rotation g_2 , and let angle ψ vary. In this way we obtain all rotations g for which the crystal direction $\vec{h}$ coincides with the sample direction $\vec{y}$. Similarly, all rotations g , for which the crystal direction $-\vec{h}$ coincides with the sample direction $\vec{y}$, are given by

$$g_1 = \left\{ \frac{3\pi}{2} + \varphi, \pi - \theta, \psi \right\}^{-1} \left\{ \frac{\pi}{2} + \eta, \chi, 0 \right\}, \quad \psi \in [0, 2\pi).$$

If we substitute expression (B1) into Eq. (10), and use the addition theorem for spherical functions on the group SO(3), we obtain

$$\begin{aligned}
\bar{P}_h(\vec{y}, g_0, \varepsilon) &= (4\pi)^{-1} \int_0^{2\pi} \left[f\left(\left\{\frac{\pi}{2} + \varphi, \theta, \psi\right\}^{-1} \left\{\frac{\pi}{2} + \eta, \chi, 0\right\}, g_0, \varepsilon\right) \right. \\
&\quad \left. + f\left(\left\{\frac{3\pi}{2} + \varphi, \pi - \theta, \psi\right\}^{-1} \left\{\frac{\pi}{2} + \eta, \chi, 0\right\}, g_0, \varepsilon\right) \right] d\psi \\
&= (4\pi)^{-1} \sum_{l=0}^{\infty} F_l(\varepsilon) \times \sum_{m,k,n=-l}^l T_l^{mk}(g_0) T_l^{kn} \left(\left\{\frac{\pi}{2} + \eta, \chi, 0\right\}^{-1} \right) \\
&\quad \times \int_0^{2\pi} \left[T_l^{nm} \left(\left\{\frac{\pi}{2} + \varphi, \theta, \psi\right\} \right) + T_l^{nm} \left(\left\{\frac{3\pi}{2} + \varphi, \pi - \theta, \psi\right\} \right) \right] d\psi \\
&= (4\pi)^{-1} \sum_{l=0}^{\infty} F_l(\varepsilon) \sum_{m,n=-l}^l T_l^{mn} \left(g_0 \left\{\frac{\pi}{2} + \eta, \chi, 0\right\}^{-1} \right) \\
&\quad \times \left[\exp \left\{ -i n \left(\frac{\pi}{2} + \varphi \right) \right\} P_l^{nm}(\cos \theta) \right. \\
&\quad \left. + \exp \left\{ -i n \left(\frac{3\pi}{2} + \varphi \right) \right\} P_l^{nm}(-\cos \theta) \right] \int_0^{2\pi} \exp \{ -i m \psi \} d\psi \\
&= (4\pi)^{-1} \sum_{l=0}^{\infty} F_l(\varepsilon) \sum_{n,m=-l}^l T_l^{mn} \left(g_0 \left\{\frac{\pi}{2} + \eta, \chi, 0\right\}^{-1} \right) \\
&\quad \times \left[\exp \left\{ -i n \left(\frac{\pi}{2} + \varphi \right) \right\} \right. \\
&\quad \left. \times \left[P_l^{nm}(\cos \theta) + (-1)^n P_l^{nm}(-\cos \theta) \right] 2\pi \delta_{m0} \right] \\
&= \frac{1}{2} \sum_{l=0}^{\infty} F_l(\varepsilon) \sum_{n=-l}^l T_l^{0n} \left(g_0 \left\{\frac{\pi}{2} + \eta, \chi, 0\right\}^{-1} \right) \exp \left\{ -i n \left(\frac{\pi}{2} + \varphi \right) \right\} \\
&\quad \times \left[P_l^{n0}(\cos \theta) + (-1)^n P_l^{n0}(-\cos \theta) \right].
\end{aligned}$$

We have $P_l^{n0}(-\cos \theta) = (-1)^{l-n} P_l^{n0}(\cos \theta)$, and thus we get

$$\bar{P}_h(\vec{y}, g_0, \varepsilon) = \frac{1}{2} \sum_{l=0}^{\infty} F_l(\varepsilon) [1 + (-1)^l] T_l^{00}(\vec{g}) = \sum_{l=0}^{\infty} F_{2l}(\varepsilon) P_{2l}(\cos \vec{\beta}),$$

where

$$\vec{g} = \{\vec{\alpha}, \vec{\beta}, \vec{\gamma}\} = g_0 \left\{ \frac{\pi}{2} + \eta, \chi, 0 \right\}^{-1} \left\{ \frac{\pi}{2} + \varphi, \theta, 0 \right\},$$

$$T_l^{00}(\vec{g}) \equiv P_l(\cos \vec{\beta}), \quad \cos \vec{\beta} = (\vec{h}, g_0 \vec{y})$$

(Vilenkin, 1965).

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