OPTIMAL CALCULATION OF ODF WITH THE CANONICAL NORMAL DISTRIBUTION ON THE ROTATION GROUP

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Macroscopic physical properties of most polycrystalline materials are controlled by orientation distribution of their grains. The orientation distribution function (ODF) of a polycrystal is seldom if ever determined directly from an experiment. Usually experimental data are represented by a set of pole figures (PFs), these latter are some integral projections of the ODF. The main problem of quantitative texture analysis is to recover ODF from its corresponding PFs. With any set of PFs the solution of this problem is non-unique. That is why some assumptions about ODF structure are necessary. We consider ODF as superposition of the canonical normal distribution (CND) on the rotation group $SO(3)$.

Keywords: Orientation distribution function; Canonical normal distribution

ROTATION PARAMETERS AND REPRESENTATION

All kinds of rotations in the 3-dimensional space form the rotation group $SO(3)$. Let a unitary representation of the group be specified, i.e. unitary operators T_g exist for any rotation $g \in SO(3)$ so that

$$\begin{aligned}T_{g_1 g_2} &= T_{g_1} T_{g_2}, \\ T_e &= I.\end{aligned}$$

If a rotation is defined by parameters (ξ_1, ξ_2, ξ_3) (where $\vec{\xi}$ coincides with the rotation axis, and $|\vec{\xi}| = \delta$ is equal to the rotation angle), then we

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get

$$T(g) \equiv T(\xi_1, \xi_2, \xi_3) = e^{\xi_1 A_1 + \xi_2 A_2 + \xi_3 A_3},$$

where A_1, A_2, A_3 are the operators of infinitesimal rotations around coordinate axes. These operators completely define the representation (Gelfand *et al.*, 1958). In the basis of the eigen vectors of A_3 operator, T_g takes the form of unitary matrix with generalised spherical functions $T_l^{mn}(g)$ as elements. If the rotation is defined by Eulerian angles $(\psi, \vartheta, \varphi)$, then we have (Vilenkin, 1991)

$$T_l^{mn}(g) = e^{-im\varphi - in\vartheta} P_l^{mn}(\cos \vartheta).$$

The parameters (ξ_1, ξ_2, ξ_3) and $(\psi, \vartheta, \varphi)$ are related by the following equations:

$$\begin{cases} \xi_1 = s\delta \sin(\vartheta/2) \cos((\psi - \varphi)/2) / \sin(\delta/2), \\ \xi_2 = s\delta \sin(\vartheta/2) \sin((\psi - \varphi)/2) / \sin(\delta/2), \\ \xi_3 = s\delta \cos(\vartheta/2) \sin((\psi + \varphi)/2) / \sin(\delta/2), \\ \cos(\delta/2) = s \cos(\vartheta/2) \cos((\psi + \varphi)/2), \\ s = \text{sign}(\cos((\psi + \varphi)/2)). \end{cases}$$

DEFINITION

Consider the canonical normal distribution (CND) on the group $SO(3)$. Let $\{T_l(g)\}$ be a set of irreducible representations of $SO(3)$. The distribution density $f(g)$ is said to be canonical normal if it admits representation of the following type (Savyolova, 1984; 1993):

$$\int_{SO(3)} T_l(g) f(g) dg = e^{\alpha_{11}(A_1')^2 + \alpha_{22}(A_2')^2 + \alpha_{33}(A_3')^2},$$

where $\alpha_{11}, \alpha_{22}, \alpha_{33}$ are non-negative constants and dg is the invariant measure on $SO(3)$,

$$dg = \sin \vartheta d\vartheta d\psi d\varphi = \frac{\sin^2(\delta/2)}{(\delta/2)^2} d\xi_1 d\xi_2 d\xi_3.$$

In this case we have the formula

$$\begin{aligned} f(g) &= \sum_{l=0}^{\infty} (2l+1) \text{Sp} (e^{\alpha_{11}(A_1^l)^2 + \alpha_{22}(A_2^l)^2 + \alpha_{33}(A_3^l)^2} e^{\xi_1 A_1^l + \xi_2 A_2^l + \xi_3 A_3^l}) \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n=-l}^l C_l^{mn} T_l^{mn}(g). \end{aligned}$$

PROPERTIES OF THE CND

1. The function $f(g)$ has the same values for the following 8 rotations:

(ξ_1, ξ_2, ξ_3) or in Eulerian angles	$(\psi, \vartheta, \varphi)$,
$(\xi_1, \xi_2, -\xi_3)$	$(2\pi - \varphi, \vartheta, 2\pi - \psi)$,
$(\xi_1, -\xi_2, \xi_3)$	$(\varphi, \vartheta, \psi)$,
$(\xi_1, -\xi_2, -\xi_3)$	$(2\pi - \psi, \vartheta, 2\pi - \varphi)$,
$(-\xi_1, \xi_2, \xi_3)$	$(\pi - \psi, \vartheta, \pi - \varphi)$,
$(-\xi_1, \xi_2, -\xi_3)$	$(\pi + \varphi, \vartheta, \pi + \psi)$,
$(-\xi_1, -\xi_2, \xi_3)$	$(\pi - \varphi, \vartheta, \pi - \psi)$,
$(-\xi_1, -\xi_2, -\xi_3)$	$(\pi + \psi, \vartheta, \pi + \varphi)$.

This property allows to reduce calculation 8 times.

2. Consider the dependence of CND on the parameters $(\alpha_{11}, \alpha_{22}, \alpha_{33})$. Now we designate $f \equiv (\alpha_{11}, \alpha_{22}, \alpha_{33}, \xi_1, \xi_2, \xi_3)$. Any permutation of distribution parameters $(\alpha_{11}, \alpha_{22}, \alpha_{33})$ causes respective permutation of rotation parameters (ξ_1, ξ_2, ξ_3) , i.e.

$$\begin{aligned} f(\alpha_{11}, \alpha_{22}, \alpha_{33}, \xi_1, \xi_2, \xi_3) &= f(\alpha_{22}, \alpha_{11}, \alpha_{33}, \xi_2, \xi_1, \xi_3) \\ &= f(\alpha_{22}, \alpha_{33}, \alpha_{11}, \xi_2, \xi_3, \xi_1) = \dots \end{aligned}$$

For example the permutation $\alpha_{11} \leftrightarrow \alpha_{22}$ is equal to the substitution $\psi \rightarrow \pi/2 - \psi$, $\varphi \rightarrow 3\pi/2 - \varphi$.

3. The CND $f(g)$ peaks at the rotation $g = e = (0, 0, 0)$ and the maximum does not depend on the order of parameters $(\alpha_{11}, \alpha_{22}, \alpha_{33})$,

$$f(0, 0, 0) = \sum_{l=0}^{\infty} (2l+1) \text{Sp } \Lambda_l,$$

where Λ_l is the diagonal form of the matrix $e^{\alpha_{11}(A_1^l)^2 + \alpha_{22}(A_2^l)^2 + \alpha_{33}(A_3^l)^2}$.

APPROXIMATION OF CND

Consider the distribution of the following type:

$$\hat{f}(g) = 1 + \sum_{l=1}^{\infty} (2l+1) e^{-\varepsilon_l^2 l(l+1)} \frac{\sin((2l+1)\hat{\delta}/2)}{\sin(\hat{\delta}/2)},$$

where

$$\hat{\delta}^2 = \tilde{\xi}_1^2 + \tilde{\xi}_2^2 + \tilde{\xi}_3^2 \quad \text{with} \quad \hat{\xi}_i = \frac{\varepsilon_l}{\sqrt{\alpha_{ii}}} \xi_i$$

and

$$\varepsilon_l^2 = \frac{1}{l(l+1)} \ln \frac{2l+1}{\text{Sp}(\Lambda_l)}.$$

The distribution function $\hat{f}(g)$ satisfies the properties 1–3. Numerical calculations reveal that $\hat{f}(g)$ approximates CND with sufficient accuracy. If the parameters $\{\alpha_{ii}\}$ are comparatively small ($\alpha_{ii} < \frac{1}{4}$), then $\hat{f}(g)$ can be replaced by the formula

$$\tilde{f}(g) = \frac{\sqrt{\pi}}{\sqrt{\alpha_{11}\alpha_{22}\alpha_{33}}} \exp\{-(\xi_1^2/\alpha_{11} + \xi_2^2/\alpha_{22} + \xi_3^2/\alpha_{33})\}.$$

The distribution $\tilde{f}(g)$ was proposed previously by Savyolova and Ivanova (1992). The numerical calculations of CND with different parameters are demonstrated in Savyolova and Davidzhan (1997).

CONCLUSION

The CND is the distribution of general kind for approximation ODF. The present work gives number of the CND properties and some approximation formulae.

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