Journal of Physics: Conference Series

Axial closed-form texture component approximating the canonical normal distribution

To cite this article: T M Ivanova 2019 *J. Phys.: Conf. Ser.* **1205** 012021

MPMM 2018 IOP Publishing
IOP Conf. Series: Journal of Physics: Conf. Series **1205** (2019) 012021 doi:10.1088/1742-6596/1205/1/012021

Axial closed-form texture component approximating the canonical normal distribution

T M Ivanova

Department of High Mathematics, National Research Nuclear University, 31 Kashirskoe Shosse, Moscow 115409, Russia

e-mail: `ivatatiana@gmail.com`

Abstract. Easily calculated texture components are necessary for solving problems of quantitative texture analysis (QTA). In the present work we obtain closed-form approximation for the axial component of the canonical normal distribution on SO(3) with central and non-central scattering.

1. Introduction

Modeling and interpreting the texture of polycrystalline materials by the component fit method is based on the use of standard functions [1]. The latter describe the shape, the position in the orientation space and the scattering of texture components. The texture components in the form of the canonical normal distribution (CND) on the rotation group SO(3) [2] are widely used in quantitative texture analysis
[3] – [6].

Let the quaternion $R[\vec{n},\omega]=\cos\frac{\omega}{2}+\vec{n}\sin\frac{\omega}{2}$ determines the rotation g about the axis $\vec{n}$ by the angle ω. The peak component of the canonical normal distribution with central scattering described by the parameter ε is given by the series [2] – [3]:

$$f^{peak}(R[\vec{n},\omega],\varepsilon)=\sum_{l=0}^{\infty}(2l+1)\exp\left(-l(l+1)\varepsilon^2\right)\frac{\sin\left((2l+1)\frac{\omega}{2}\right)}{\sin\frac{\omega}{2}}. \tag{1}$$

The corresponding axial component with the axis $\vec{n}_A$ can be represented by the series of Legendre polynomials

$$f^{axial}(\vec{n}_A,g,\varepsilon)=\sum_{l=0}^{\infty}(2l+1)\exp\left(-l(l+1)\varepsilon^2\right)P_l\left(\left(g\vec{n}_A,\vec{n}_A\right)\right), \tag{2}$$

Application of texture components (1) – (2) in the solution of the QTA problems is associated with large computational costs, as well as the necessity of truncating the series depending on the sharpness of the texture [4] – [6].

A computationally convenient approximation for the distribution (1) was obtained in [7]:

$$f_{approx}^{peak}(R[\vec{n},\omega],\varepsilon^2)=\frac{\sqrt{\pi}}{\varepsilon^3}\cos^{-4}\left(\frac{\omega}{2}\right)\exp\left\{-\frac{1}{\varepsilon^2}\tan^2\left(\frac{\omega}{2}\right)\right\}. \tag{3}$$

In the case of a non-central character of the scattering, the canonical normal distribution on SO (3) is represented by the triple series of generalized spherical harmonics [2]:

$$f^{peak}(g,\vec{\varepsilon})=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\sum_{n=-l}^{l}C_l^{mn}(\vec{\varepsilon})T_l^{mn}(g).$$

The coefficients of the series can be found only numerically, but its approximation has a rather simple form [7]:

$$f_{approx}^{peak}(g,\vec{\varepsilon})=$$

$$=\frac{\sqrt{\pi}}{\varepsilon_1\varepsilon_2\varepsilon_3\cos^4\left(\frac{\omega}{2}\right)}\exp\left\{-\frac{\tan^2\left(\frac{\beta}{2}\right)}{\cos^2\left(\frac{\alpha+\gamma}{2}\right)}\left[\frac{\sin^2\left(\frac{\alpha-\gamma}{2}\right)}{\varepsilon_1^2}+\frac{\cos^2\left(\frac{\alpha-\gamma}{2}\right)}{\varepsilon_2^2}\right]-\frac{\tan^2\left(\frac{\alpha+\gamma}{2}\right)}{\varepsilon_3^2}\right\}, \tag{4}$$

where $\vec{\varepsilon}=\{\varepsilon_1,\varepsilon_2,\varepsilon_3\}$ is a vector of scattering parameters, $\{\alpha,\beta,\gamma\}$ are the Euler angles of the rotation g, associated with the quaternion $R[\vec{n},\omega]$ by the relation

$$\cos\frac{\omega}{2}+\vec{n}\sin\frac{\omega}{2}=\cos\frac{\beta}{2}\cos\frac{\alpha+\gamma}{2}+\sin\frac{\beta}{2}\left(\vec{i}\sin\frac{\alpha-\gamma}{2}+\vec{j}\cos\frac{\alpha-\gamma}{2}\right)+\vec{k}\cos\frac{\beta}{2}\cos\frac{\alpha+\gamma}{2}.$$

However, the texture contains not only the peak components generally. Usually, the model includes axial components as well. And quite often the texture is described by them only. This paper is devoted to obtaining a convenient approximation of the axial component for the canonical normal distribution.

2. The relationship between the peak and axial components

The axial component is invariant with respect to rotations about a fixed axis. It is obtained by averaging the peak component over all possible rotations around the axis. If these rotations are represented by quaternion $R_A=\cos\frac{\omega_A}{2}+\vec{n}_A\sin\frac{\omega_A}{2}$, then

$$f^{axial}(\vec{n}_A,R[\vec{n},\omega],\varepsilon)=\frac{1}{2\pi}\int_0^{2\pi}f^{peak}(R_A^{-1}R,\varepsilon)\,d\omega_A. \tag{5}$$

As a result of averaging, $\vec{n}_A$ becomes the axis of the texture.

3. Approximating function for the axial component of the central normal distribution

The approximation of the axial component of the canonical normal distribution (2) is obtained by applying the averaging to the distribution (3). In this case, as an argument of the peak component, we take the angle $\tilde{\omega}$, corresponding to the product of the rotations $g_A^{-1}g$:

$$\cos\frac{\tilde{\omega}}{2}=\cos\frac{\omega_A}{2}\cos\frac{\omega}{2}+(\vec{n}_A,\vec{n})\sin\frac{\omega_A}{2}\cos\frac{\omega}{2}. \tag{6}$$

Substituting (6) into (3) and performing the integration in (5), we obtain

$$f_{approx}^{axial}\left(\vec{n}_A, R\left[\vec{n},\omega\right],\varepsilon\right)=\frac{\left\{\frac{1}{\varepsilon^2}+\frac{1}{2}\left(1-\sin^2\frac{\omega}{2}\cdot\left[\vec{n}_A,\vec{n}\right]^2\right)\right\}}{\left\{\left(1-\sin^2\frac{\omega}{2}\cdot\left[\vec{n}_A,\vec{n}\right]^2\right)\right\}^{3/2}}\exp\left\{-\frac{1}{\varepsilon^2}\frac{\sin^2\frac{\omega}{2}\cdot\left[\vec{n}_A,\vec{n}\right]^2}{1-\sin^2\frac{\omega}{2}\cdot\left[\vec{n}_A,\vec{n}\right]^2}\right\}, \quad (7)$$

In terms of rotation g , the approximating distribution (7) takes the form

$$f_{approx}^{axial}\left(\vec{n}_A, g,\varepsilon\right)=\frac{\left\{\frac{1}{\varepsilon^2}+\frac{1+\left(g\,\vec{n}_A,\vec{n}_A\right)}{4}\right\}}{\left\{\frac{1+\left(g\,\vec{n}_A,\vec{n}_A\right)}{2}\right\}^{3/2}}\exp\left\{-\frac{1}{\varepsilon^2}\frac{1-\left(g\,\vec{n}_A,\vec{n}_A\right)}{1+\left(g\,\vec{n}_A,\vec{n}_A\right)}\right\}, \quad (8)$$

If the axis of rotation $\vec{n}_A=\left(0,0,1\right)$, then $\left(g\,\vec{n}_A,\vec{n}_A\right)=\cos\beta,$ thus

$$f_{approx}^{axial}\left((0,0,1),\ g,\ \varepsilon\right)=\frac{\left\{\frac{1}{\varepsilon^2}+\frac{1}{2}\cos^2\frac{\beta}{2}\right\}}{\cos^3\frac{\beta}{2}}\exp\left\{-\frac{1}{\varepsilon^2}\tan^2\frac{\beta}{2}\right\}. \quad (9)$$

4. Approximation of the axial component with non-center scattering

For the non-central distribution (4), the most interesting is the case, when $\vec{n}_A=\left(0,0,1\right)$. Averaging (4) over all possible rotations about this axis, we obtain

$$f_{approx}^{axial}\left((0,0,1),\ g,\ \vec{\varepsilon}\right)=\frac{1}{\varepsilon_1\varepsilon_2\varepsilon_3}\frac{\left\{1+\frac{1}{2A}+\frac{B^2}{A^2}\right\}}{\sqrt{A}\cos^4\frac{\beta}{2}}\exp\left\{-\frac{AC-B^2}{A}\right\}, \quad (10)$$

with

$$A=\left(\frac{\cos^2\gamma}{\varepsilon_1^2}+\frac{\sin^2\gamma}{\varepsilon_2^2}\right)\tan^2\frac{\beta}{2}+\frac{1}{\varepsilon_3^2},\ B=\left(\frac{\sin^2\gamma}{\varepsilon_1^2}+\frac{\cos^2\gamma}{\varepsilon_2^2}\right)\tan^2\frac{\beta}{2},\ C=\left(\frac{1}{\varepsilon_2^2}-\frac{1}{\varepsilon_1^2}\right)\sin\gamma\cos\gamma\tan^2\frac{\beta}{2}.$$

Note, that in case $\varepsilon_1=\varepsilon_2=\varepsilon_3=\varepsilon,$ the distribution (10) goes into (9).

5. Conclusion

In the paper, distributions (7) – (10) approximating the axial component of the canonical normal distribution with the central and non-central scattering are obtained. They obey closed form and are convenient in calculations. These distributions can be recommended as standard functions for solving problems of quantitative texture analysis.

It should be noted that everywhere above it was assumed that the maximum of the distribution corresponds to zero rotation. The displacement of the maximum to the point g_0 in the orientation space can be achieved by replacing $g \to g_0^{-1} g$, and respectively, $R \to R_0^{-1} R$.

References

[1] Bunge H J 1982 *Texture Analysis in Material Science* (Butterworths:London)
[2] Nikolayev D I and Savyolova T I 1997 Normal distribution on the rotation group SO(3) , *Text. Microstruct*. **29** 201–33
[3] Bucharova T I and Savyolova T I 1993 Application of normal distribution on SO(3) and S2 for orientation distribution function approximation *Text. Microstruct*. **23** 161–176
[4] Ivanova T M and Savelova T I 2006 Robust method of approximating the orientation distribution function by canonical normal distributions *Phys. Met. Metallog*. 101 N2 114–118
[5] Ivanova T M and Serebryany V N 2017 Methods of recovering orientation distribution function using texture components with a circular normal distribution Indust. Lab. 83 I-1 43–47
[6] Ivanova T M Savyolova T I and Sypchenko M V 2010 The modified component method for calculation of orientation distribution function from pole figures *Inverse Problems in Science and Engineering* 18 N1 163–171
[7] Ivanova T M and Nikolayev D I 2001 New Standard Function for Quantitative Texture Analysis *Phisica Status Solidi* 228 N3 825–836