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Applying Gaussian Distributions on SO(3) for Modeling the Texture and Predicting the Properties of Texturized Polycrystalline Materials

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Abstract. This paper considers a quantitative description of the crystallographic texture. When the crystallographic texture is modeled, the generalized Gaussian distribution is applied on Riemannian manifolds. A simple model of the orientation distribution function (ODF) is obtained, which corresponds to the Gaussian distribution of the axial crystallographic texture. It is demonstrated that an equally probable distribution of crystallographic axes and an ideal axial texture are realized as special cases of the ODF model. An anisotropy evaluation of elastic modulus is carried out. The indicatrix transformation of Young's modulus is demonstrated.

DESCRIPTION OF CRYSTALLOGRAPHIC TEXTURE

It has been known that a quantitative description of the crystallographic texture can be realized in different ways: following the method of specific volumes, by means of the orientation distribution function (ODF) as series over the generalized spherical functions, and also through the use of some model representations of ODF. The simplest model distributions to be utilized for describing axial textures can be the wrapped normal distribution with a density and the von Mises distribution [1]:

$$f(\theta)=\frac{1}{\sigma\sqrt{2\pi}}\sum_{k=-\infty}^{+\infty}\exp\left\{-\frac{\theta+2\pi k}{2\sigma^2}\right\},\ g(\theta,\mu,k)=\frac{1}{2\pi I_0(k)}\exp\{k\cos(\theta-\mu)\},\quad |\mu|<+\infty, k>0,$$

where $I_0(k)$ is a modified Bessel function of the zeroth order.

The ODF shows how many times the distribution density of the angle θ in the texturized state is as great as the density in a non-texturized polycrystal. That is,

$$F(\theta)=f(\theta)\frac{\sin\theta}{2}.$$

The wrapped normal distribution and the von Mises distribution do not possess all the properties characteristic of the normal distribution on the straight line. General results have been reported in [1-6] as distribution representations on group S0(3). When modeling a crystallographic texture, a significant generalization of the description can be achieved by using the generalized Gaussian distribution on Riemannian manifolds [7].

Following the ideas advanced in [7], a quite simple ODF model corresponding to the Gaussian distribution of the axial crystallographic texture can be represented in the form

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$$F(\theta)=\frac{e^{-\gamma\theta^2}}{\int_0^{\pi}\frac{\sin\theta}{2}e^{-\gamma\theta^2}d\theta}\,.$$

If $\gamma\to 0$, then $F(\theta)\to 1$ (an equally probable distribution of the crystallographic axes is realized); at $\gamma\to\infty$, $F(\theta)\to\delta(\theta)$ (an ideal axial texture is realized). At various values of γ, the ODF is displayed in Fig. 1.

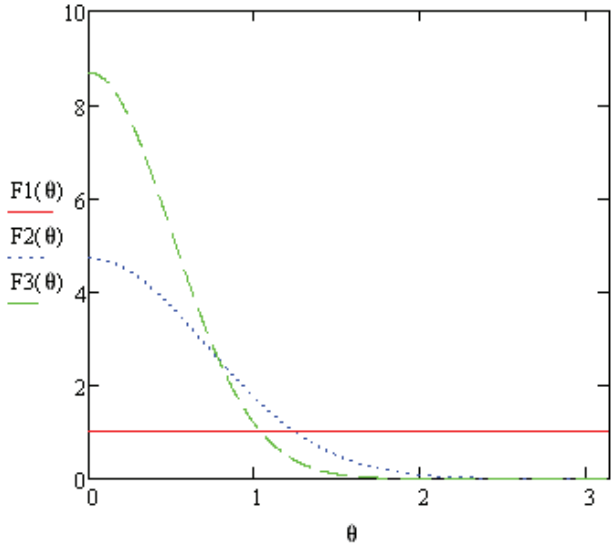

FIGURE 1. ODF curves: $F1(\theta)\quad(\gamma=0)$; $F2(\theta)\quad(\gamma=1)$; $F3(\theta)\quad(\gamma=2)$

EVALUATION OF PHYSICAL AND MECHANICAL ANISOTROPY

Within the frameworks of the method for constructing direct pole figures used for the analysis of the texture of polycrystalline materials, the resulted relative intensity is similar to the ODF, and it can be applied for carrying out the evaluation of their physical and mechanical anisotropy.

In each point of the micro-anisotropic continuum, the strains and stresses are correlated with the generalized Hooke's law equations [8]

$$\varepsilon_{ij}=s_{ijmn}\sigma_{mn}$$

where σ_{ij} denotes the components of the random stress tensor, ε_{ij} denotes the components of the random strain tensor, s_{ijmn} is the components of the random compliance tensor, over the indexed values, here and further summation is implied over the set from 1 to 3.

The procedure of averaging the compliance tensor can be carried out in two steps. Firstly, averaging is performed over the rotation angle around the preferred orientation axis $\langle uvw\rangle$, and then averaging is performed that allows for the dispersion of that axis position.

At the first step, the averaged compliance coefficients are found for a polycrystal having an ideal axial texture determined by the crystallographic direction $\langle uvw\rangle$.

$$\langle s''_{11}\rangle=s'_{11}-s(1+3\Delta)/4,\quad \langle s''_{33}\rangle=s'_{11}-2s\Delta,\quad \langle s''_{13}\rangle=s'_{12}+s\Delta,\quad \langle s''_{12}\rangle=s'_{12}+s(1-\Delta)/4,\quad \langle s''_{44}\rangle=s'_{44}+4s\Delta,$$

where $s=s'_{11}-s'_{12}-0.5s'_{44}$, $\Delta=\dfrac{u^2v^2+v^2w^2+w^2u^2}{\left(u^2+v^2+w^2\right)^2}$, s'_{ij} denotes the crystallite compliance coefficients.

Further averaging to allow for the dispersion of the axial texture can be carried out on the condition that a polycrystal with the axial texture and cubic symmetry of the crystal lattice has the compliance coefficients that, in

Royce's approximation, coincide with the compliance coefficients of a polycrystal with the axial texture and the hexagonal symmetry of the grain crystal lattice:

$$s_{11}^R = s'_{11} - s(1+0.6A)/4, \quad s_{33}^R = s'_{11} - 0.4s\,A, \quad s_{13}^R = s'_{12} + 0.2s\,A, \quad s_{12}^R = s'_{12} + s(1-0.2A)/4, \quad s_{44}^R = s'_{44} + 0.8s\,A,$$

where $A = 5\Delta + 5(1-5\Delta)q/4$; and the q parameter determines dispersion of the texture,

$$q = \int_0^{\pi} \left(4\sin^2\theta - \frac{7}{2}\sin^4\theta\right) F(\theta)\frac{\sin\theta}{2}\,d\theta\,.$$

Finding the integral results in $q = 4/5$ and $A = 1$. The resulted expressions for the averaged compliance coefficients and elasticity modules coincide with the known expressions for quasi-isotropic polycrystals. As seen, isotropy occurs at $q = 4/5$ and $\Delta = 1/5$. Such effects can appear because of creating a "special" dispersion of the texture or due to selecting the preferred orientation axis. The isotropy of molybdenum wire having a $\langle 320\rangle$ texture can be taken as such an example [9]. In this case, calculations result in the value $A = 1.06$.

ELASTIC MODULUS

Anisotropy evaluation of Young's modulus, which is regarded as the most common characteristic of the deformation of solids, can be obtained using the following relation:

$$E^{-1}(\theta) = s_{11} - s\left(\frac{55+9A}{160} - \frac{1-A}{8}\cos 2\theta - \frac{7(1-A)}{32}\cos 4\theta\right).$$

Figure 2 displays the indicatrix transformation of Young's modulus for a texturized polycrystal of copper as the parameter A changes in the limits from 0 to $5/3$. The elasticity coefficients are $s'_{11} = 1.498$; $s'_{44} = 1.326$; $s'_{12} = -0.629$ (in 10^{-11} Pa).

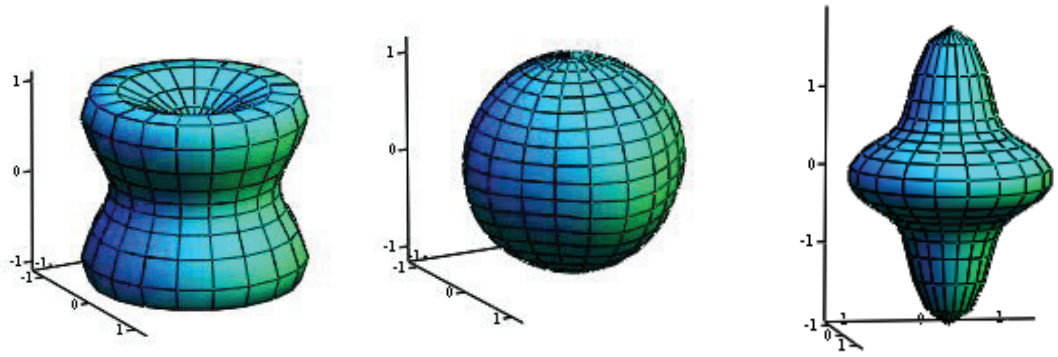

FIGURE 2. Indicatrix transformation of Young's modulus for a texturized polycrystal of copper with a changing texture: $A = 0, \quad A = 1, \quad A = 5/3$

CONCLUSIONS

The crystallographic texture is modeled with the use of the generalized Gaussian distribution on Riemannian manifolds. In the explicit form, the ODF model is presented, which corresponds to the Gaussian distribution of the axial texture. By example of a copper polycrystal, the qualitative change in the Young's modulus indicatrix is demonstrated with the changing texture.

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