

A NEW APPROACH TO DESCRIBING THREE-DIMENSIONAL ORIENTATION DISTRIBUTION FUNCTIONS IN TEXTURED MATERIALS

II. Model ODF For Rolling Textures

V. N. DNIEPRENKO AND S. V. DIVINSKII

*Institute of Metal Physics, Ukrainian Academy of Sciences,
Prospekt Vernadskogo 36, Kiev-142, 252680, Ukraine*

Sections of a three-dimensional Orientation Distribution Function (ODF) for the α -Fe rolling texture typical for most b.c.c. metals have been constructed on the basis of the proposed new method for ODF simulation through the representation of a crystallite orientation by nine rotations, only three of which are varied for a given component. The description of texture by superposition of partial fibre components is used. A comparison of such a model ODF with an ODF reconstructed from experimental pole figures by series expansion is presented. As a result all really encountered textures can be simulated by variation of the crystallite spread parameters, texture axis positions, and predominant preferred orientations in terms of a common approach.

KEY WORDS: Model ODF partial fibre components anisotropic spread orientation tubes.

INTRODUCTION

In the first paper of this series (Dnieprenko, Divinski (1993)) (further signed by I) a new approach to simulate pole figures by means of Orientation Distribution Functions (ODF) given in analytical form has been suggested. Other ODF simulation methods existing at present. e.g. of Bunge (1969), Matthies (1969), Bukharova, Kapcherin, Nicolaev, Papirova, Savelova, Shkuropatenko (1984), Jura (1988), can be treated as particular cases of the model of I. Namely both "ideal" textures with a spherical spread relative to the positions of some preferred orientations (as in Bunge (1969), Matthies (1969), Bukharova *et al.* (1984)) and axial components with an isotropic spread around some preferred axes (as in Jura (1988)) may be simulated in the presented method by a variation of spread parameters. In this cases the difference in the analytical form of the ODF in Dnieprenko *et al.* (1993) and in Bunge (1969), Matthies (1969), Bukharova *et al.* (1984) and Jura (1988) does not considerably affect the pole density distribution pattern.

The difference of the model proposed in I consists in the representation of the ODF as a sum of partial fibre components. To prove the advantage of the proposed approach a comparison of such a model ODF with an ODF obtained through reconstruction from experimental pole figures by series expansion should be made. This is the object of the present study.

ODF For Typical Rolling Textures of B.C.C. Metals

As an example, let us consider the rolling texture of α -Fe treated in I which has a typical pole figure pattern for b.c.c. metals. Based on the component analysis described in I we may find the $f^M(G)$ ODF in coordinates of the angles $G = (\Psi_0, \theta_0, \Phi_0, \gamma_1, \gamma_2, \gamma_3, \Psi_1, \theta_1, \Phi_1)$. Although in the suggested model a crystallite orientation is described by a large set of angles G , the spread of a texture component itself is formed by rotations depending only on three of them $g_\gamma = (\gamma_1, \gamma_2, \gamma_3)$. Rotations $g_0 = (\Psi_0, \theta_0, \Phi_0)$ and $g_1 = (\Psi_1, \theta_1, \Phi_1)$ are necessary for that the spread of the model texture component would correspond to the preferred orientation $(hk1)[uvw]lu'v'w'l$ where the notation $lu'v'w'l$ is introduced in Dneprenko *et al.* (1993) for indicating of the crystallographic direction of the texture axis. Note that g_γ is determined in a coordinate system connected with the texture axis of the partial fibre component. Transformation to this coordinate system is given by the preceding rotations g_0 .

The approach allows to describe consistently the spread of the texture components relative to the axes of their formation. At the same time, in the traditional texture analysis the angles Φ_1, Φ_0, Φ_2 are used to describe the orientation of crystallites in a coordinate system connected with some external directions of the sample. This is the main different feature of the present model in comparison with earlier proposed ones.

To describe the rolling textures by an ODF $f^M(G)$ depending only on the spread-forming angles $g_\gamma = (\gamma_1, \gamma_2, \gamma_3)$ we will use a function

$$f^M(\gamma_1, \gamma_2, \gamma_3) = A \exp \left\{ - \frac{\gamma_2^2}{2\sigma_1^2} \right\} \times \exp \left\{ - \frac{1}{2} \left(\frac{|\gamma_1 + \gamma_3| - \sigma_3 + |\sigma_3 - |\gamma_1 + \gamma_3||}{2\sigma_2} \right)^2 \right\}. \quad (1)$$

proposed in I. Here σ_1, σ_2 , and σ_3 are parameters of spread of the given texture components; and A is the normalization factor.

Taking expression (1) and relation (2) in I we can determine $f(g_B)$ in the space of Eulerian angles $g_B = (\Phi_1, \Phi, \Phi_2)$. In a general form we can write:

$$f(\Phi_1, \Phi, \Phi_2) = \sum_{k=1}^N \frac{P_k}{M_k} \sum_{l=1}^{M_k} f^M(\gamma_1^{(kl)}, \gamma_2^{(kl)}, \gamma_3^{(kl)}), \quad (2)$$

where $\sum_{k=1}^N p_k = 1$, p_k are the volume fractions of the texture components; N is its number; $l=1, \dots, M_k$ is the index consistently numbering the equivalent orientations in the texture component; M_k is the number of these equivalent orientations. Values of angles $g_\gamma^{(kl)} = (\gamma_1^{(kl)}, \gamma_2^{(kl)}, \gamma_3^{(kl)})$ may be found as follows:

$$g_\gamma^{(kl)} = [g_0^{(kl)}]^{-1} \cdot g_B \cdot [g_1^{(kl)}]^{-1}. \quad (3)$$

Now, only the particular forms of $g_0^{(kl)}$ and $g_1^{(kl)}$ for every texture component are needed to obtain a solution of the corresponding trigonometric equations (3).

The α -Fe rolling texture component $\{001\}\langle 110\rangle\langle 110\rangle$ has four ODF maxima in the region $0 \leq \varphi_1, \Phi, \varphi_2 \leq \pi/2$. Three such peaks correspond to the component $\{111\}\langle \bar{1}\bar{1}2\rangle\langle 221\rangle$. For the texture maximum $(100)[0\bar{1}1]0\bar{1}11$ we have:

$$g_0 = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} \end{vmatrix}, \quad g_1 = \begin{vmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{vmatrix} \quad (4)$$

and

$$\begin{cases} \sin\gamma_1 \sin\gamma_2 = [-\cos\varphi_2 \sin\Phi + \cos\Phi]/\sqrt{2} \\ \sin\gamma_3 \sin\gamma_2 = \cos\varphi_1 \cos\Phi - \sin\varphi_1 \sin\varphi_2 \cos\Phi \\ \cos\gamma_2 = [-\cos\varphi_1 \sin\varphi_2 + \sin\varphi_1 \cos\varphi_2 \cos\Phi + \sin\varphi_1 \sin\Phi]/\sqrt{2} \end{cases} \quad (5)$$

According to relation (3) the following expressions correspond to the maximum $(111)[\bar{1}\bar{1}2]\langle 221\rangle$:

$$g_0 = \begin{vmatrix} -1/\sqrt{2} & -1/3\sqrt{2} & 2/3 \\ 1/\sqrt{2} & -1/3\sqrt{2} & 2/3 \\ 0 & 4/3\sqrt{2} & 1/3 \end{vmatrix}, \quad g_1 = \begin{vmatrix} 0 & -1 & 0 \\ 5/3\sqrt{3} & 0 & 2/3\sqrt{6} \\ -2/3\sqrt{6} & 0 & 5/3\sqrt{3} \end{vmatrix} \quad (6)$$

and

$$\begin{aligned} \sin\gamma_1 \sin\gamma_2 &= [2\{\sin\varphi_2(\cos\varphi_1 - \sin\varphi_1) + \cos\varphi_2 \cos\Phi(\cos\varphi_1 + \sin\varphi_1)\} + \cos\varphi_1 \sin\Phi]/3 \\ \sin\gamma_3 \sin\gamma_2 &= [\cos\varphi_1(\cos\varphi_2 - \sin\varphi_2) - \sin\varphi_1 \cos\Phi(\sin\varphi_2 + \cos\varphi_2)]/3\sqrt{3} - \\ &\quad - 5\sin\Phi(\sin\varphi_2 - \cos\varphi_2)]/3\sqrt{6} \\ \cos\gamma_2 &= -2[2\cos\varphi_1(\cos\varphi_2 - \sin\varphi_2) - 2\sin\varphi_1 \cos\Phi(\cos\varphi_2 + \sin\varphi_2)] + \\ &\quad + \sin\varphi_1 \sin\Phi]/9\sqrt{6} + 5[2\sin\Phi(\cos\varphi_2 + \sin\varphi_2) + \cos\Phi]/9\sqrt{3} \end{aligned} \quad (7)$$

Similar expressions for the remaining maxima can be found in a similar manner. The model ODF $f(g_B)$ with the texture parameters given in Table 1 is presented in Figure 1a. Its corresponding $f(g_B)$ obtained from experimental pole figures $\{200\}$, $\{110\}$, and $\{222\}$ using the method of series expansion (with even terms only) is shown in Figure 1b. In Figure 1c the even part of the model $f(g_B)$ is shown, where only coefficients C_1^{mn} with even l are used. The coincidence of Figure 1c and Figure 1b (as Figure 5a,b and Figure 1a,c in I) leads to the conclusion that the proposed ODF simulation method is applicable to the description of real rolling textures.

It should be noted that not all non-ghost maxima on ODF sections correspond to independent texture components. For example, the maxima belonging to the $\{112\}\langle 110\rangle$ orientation are pointed out as separate components for α -Fe rolling texture by Hu (1980). However, from the concept of partial fibre components it is clear that the local rise of orientation density in $\{112\}\langle 110\rangle$ regions is due to an overlapping of the "tails" of the two main partial fibre components $\{001\}\langle 110\rangle\langle 110\rangle$ and $\{111\}\langle \bar{1}\bar{1}2\rangle\langle 221\rangle$. Figure 2 shows the formation of a maximum in the region of the overlapping for the section of the model ODF by a $\varphi_2 = 45^\circ$ plane.

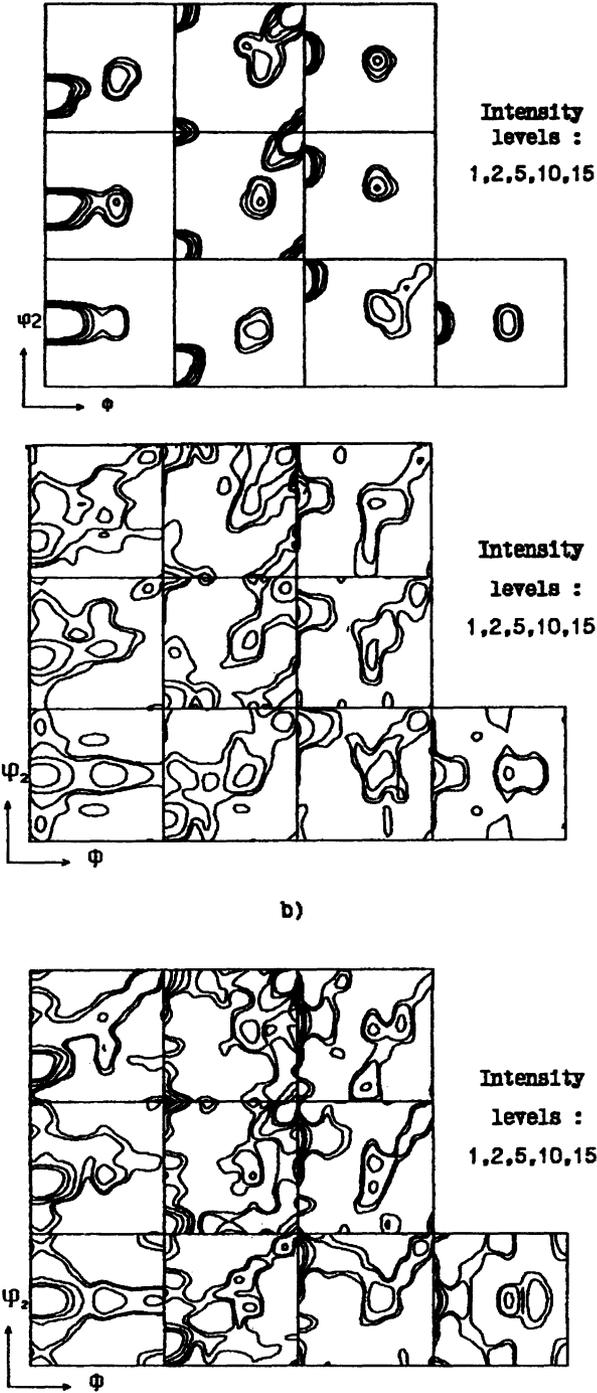


Figure 1 a) model ODF and b) even ODF reconstructed from experimental pole figures by series expansion for α -Fe rolling texture, c) even part of the model ODF.

Table 1 The ODF parameters for modeling α -Fe rolling texture

k	1	ideal orientation			Ψ_0	θ_0	φ_0	Ψ_1	θ_1	φ_1	P_k	σ_1	σ_2	σ_3
		hk1	uvw	u'v'w'										
1	1	001	$\bar{1}\bar{1}0$	$\bar{1}\bar{1}0$	$\pi/2$	$\pi/2$	$5\pi/4$	$\pi/2$	$\pi/2$	$\pi/2$	0.66	0.067	0.222	0.12
	2	100	$0\bar{1}1$	$0\bar{1}1$	π	$\pi/4$	π	$\pi/2$	$\pi/2$	$\pi/2$				
	3	001	$\bar{1}\bar{1}0$	$\bar{1}\bar{1}0$	$\pi/2$	$\pi/2$	$3\pi/4$	$\pi/2$	$\pi/2$	$\pi/2$				
	4	010	101	101	π	$\pi/4$	$\pi/2$	$\pi/2$	$\pi/2$	$\pi/2$				
2	1	111	$\bar{1}\bar{1}2$	221	π	1.23	$\pi/4$	$-\pi/2$	0.28	0	0.34	0.080	0.044	0.44
	2	111	$\bar{1}2\bar{1}$	212	1.89	0.84	1.11	$\pi/2$	0.28	$-\pi$				
	3	111	$2\bar{1}\bar{1}$	122	1.25	0.84	0.46	$-\pi/2$	0.28	0				

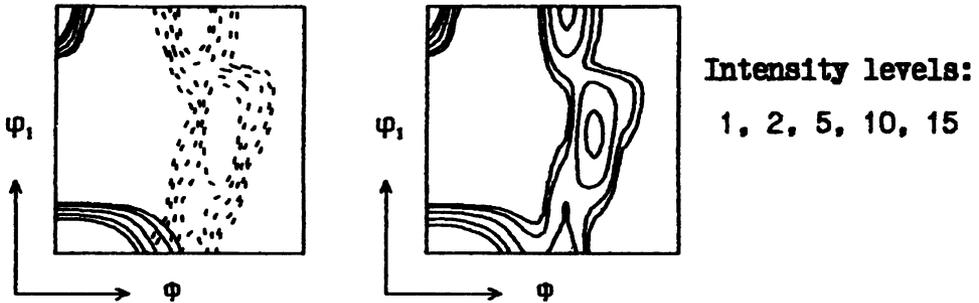


Figure 2 The section $\varphi_2=45^\circ$ of the model ODF for α -fe rolling texture. Separate components are: $\{001\}\langle 110\rangle|110|$ (—) and $\{111\}\langle \bar{1}\bar{1}2\rangle|221|$ (. . .). a) the separate components, b) their superposition

CONCLUSIONS

The crystallite orientation distribution function was found on the basis of the concept of partial fibre components. This technique allows to describe in a common manner the whole variety of spreads of preferred orientations, from a single crystal to a random polycrystal. The capabilities of this universal model ODF are illustrated by Figure 3. which presents corresponding schematic pole figures $\{100\}$ and some sections of the model ODF. Namely, the proposed model ODF (1) allows to describe all possible types of texture:

- 1) quasi single crystal ones at $\sigma_1, \sigma_2, \sigma_3 \rightarrow 0$ (Figure 3a);
- 2) with spherical spread around the maxima at $\sigma_1 = \sigma_2 \neq 0, \sigma_3 = 0$ (Figure 3b);
- 3) with anisotropical spread typical for partial fibre textures, including orientation tubes, at $\sigma_2 + \sigma_3 > \sigma_1 \neq 0$ (Figure 3c);

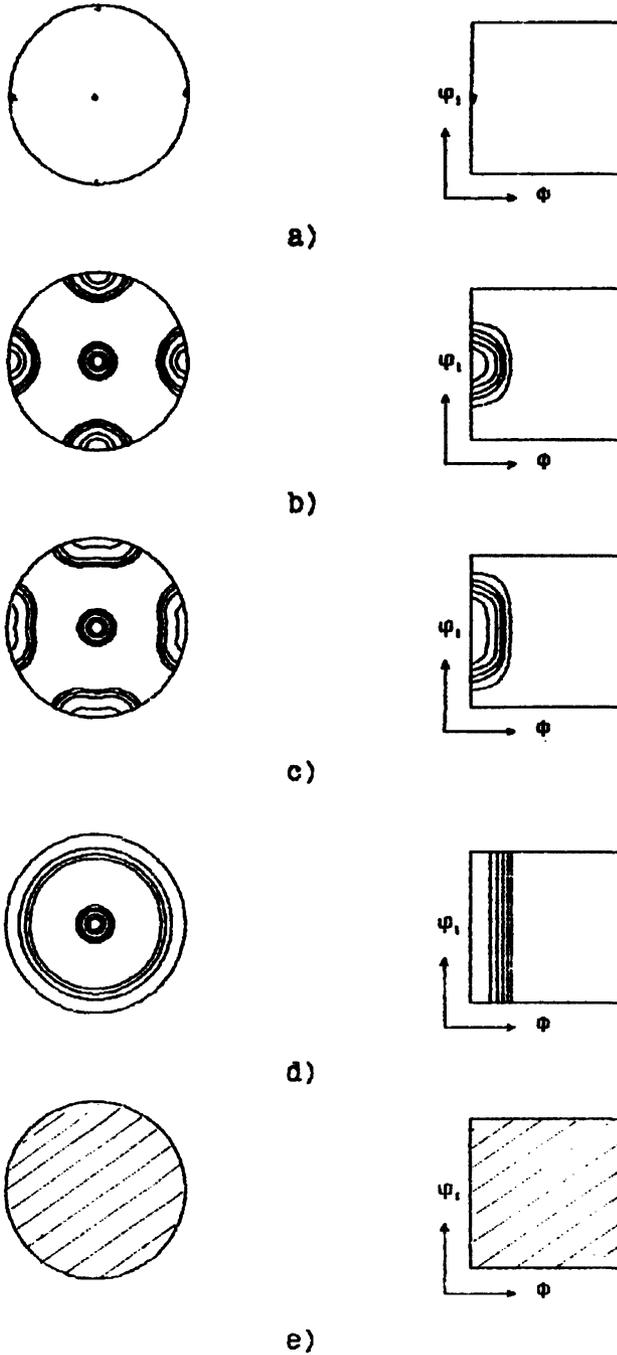


Figure 3 Schematic pole figures $\{100\}$ and sections by $\varphi_2 = \varphi_2^0$ plane of model ODFs. Values of parameters are : a) $\sigma_1 = \sigma_2 = \sigma_3 = 0$, $\varphi_2^0 = 45^\circ$; b) $\sigma_1 = \sigma_2 \neq 0$, $\sigma_3 = 0$, $\varphi_2^0 = 45^\circ$; c) $\sigma_2 + \sigma_3 > \sigma_1 \neq 0$, $\varphi_2^0 = 45^\circ$; d) $\sigma_1 \neq 0$, $\sigma_2 \rightarrow \infty$, $\varphi_2^0 = 45^\circ$; e) $\sigma_1, \sigma_2, \sigma_3 \rightarrow \infty$, $\varphi_2^0 = 45^\circ$.

- 4) fibre ones at $\sigma_2 \rightarrow \Phi$ and arbitrary σ_1, σ_3 (Figure 3d);
- 5) the random one with isotropic pole density distribution at $\sigma_1, \sigma_2 \rightarrow \Phi$, (Figure 3e).

Variant 2) provides qualitatively the same results as the techniques of Bunge (1969) or Matthies (1980). Variant 4) is similar to the method used by Jura (1988). Variant 3) is a general case of the present model introducing a different feature of ODF simulation. This expands the scope of ODF simulation and in some cases allows to describe more adequately the orientation distributions observed.

Despite a great number of variables used in the description of crystallite orientations, a clear physical meaning of every angle makes an application of our method quite simple. The model ODF is based on the concepts of texture spread formation relative to a selected direction, the texture axis. Since this concept provides a good agreement with real textures, we suggest a description of preferred orientations (hkl)[uvw] supplemented by the indication of a texture axis $lu'v'w'$.

At last it should be noted that only one of the symmetrically equivalent rotation sets g_0 and their corresponding g_1 have to be found to simulate pole figures for a texture component (hkl)[uvw] $lu'v'w'$, although a number of maxima corresponds to the components in the ODF.

References

1. Bukharova, T. I., Kapcherin, A. S., Nicolaev, A. U., Papirov, I. I., Savelova, T. I. and Shkuropatenko, V. A. (1984). *Fiz. Metallov i Metallovedenie*, **65**, 934.
2. Bunge, H. J. (1969). *Mathematische Methoden der Texturanalyse*. Akademie-Verlag, Berlin.
3. Dnieprenko, V. N. and Divinskii, S. V. (1993). *Texture and Microstructure*.
4. Hu, H. (1980). *Texture Cryst. Sol.*, **4**, 13.
5. Jura, J. (1988). *Bull. Polish Acad. of Sci.*, **36**, 183.
6. Matthies, S. (1980). *Phys. Stat. Sol. (b)*, **101**, K111.