TEXTURE ANALYSIS BY MEANS OF MODEL FUNCTIONS

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The conception of texture components is widely used in texture analysis. Mostly it is used to describe the orientation distribution function (ODF) qualitatively, and there are only a few special functions used to provide texture component calculations.

This paper attempts to introduce another model function describing common texture components and giving a compromise between universality and computational efficiency.

KEY WORDS Texture analysis, model function, normal distribution, component fit.

1. CENTRAL FUNCTIONS

The very first model ODF introduced into texture analysis has the form (Bunge, 1969):

$$f^{BG}(g) = S_0 \exp -(\omega/\omega_0)^2 \quad (1)$$

with ω —the orientation distance $|gg_0^{-1}|$. It's series expansion coefficients are expressed as follows:

$$\begin{aligned} C_l^{mn} &= a_l T_l^{mn}(g_0) \\ a_l &= c_l - c_{l+1} \\ c_l &= \frac{1}{\sqrt{4\pi}} S_0 \omega_0 \exp(-l^2 \omega_0^2/4) \end{aligned} \quad (2)$$

There are no analytically closed expressions for pole figure values available, so they have to be calculated in terms of a series expansion.

The “standard distributions”, introduced in Matthies (1982) supply analytically closed expressions for ODF and pole figure values as well as C_l^{mn} coefficients:

$$\begin{aligned} f^{SG}(g) &= N(S) \exp(S \cos \omega) \\ S &= \ln(2)/[2 \sin^2(b_{FWHM}/4)] \\ N(S) &= [I_0(S) - I_1(S)]^{-1} \\ C_l^{m,n} &= C_l(S) D_{m,n}^{l*}(g_0^{-1}) \\ C_l(S) &= N(S) [I_l(S) - I_{l+1}(S)] \\ \mathcal{P}_{\tilde{h}_i}(\vec{y}) &= N(S) I_0(S(1+z)/2) \exp(S(z-1)/2) \\ z &= \tilde{h}_i g_0 \vec{y} \end{aligned} \quad (3)$$

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(I_n —modified Bessel functions). Note, that due to the presence of $\cos \omega$ this function shows correct behavior near $\omega = \pi$ for big halfwidths, too.

2. FIBRE TEXTURES

From (3) a model function describing fibre components has been derived, which is characterized by a crystal direction $\vec{h}$ being parallel to a direction in sample coordinate system $\vec{n}$:

$$\begin{aligned}
 f^{SF}(g) &= N(S) \exp(S\vec{h} \cdot g\vec{n}) \\
 S &= \ln(2)/[2 \sin^2(b_{FWHM}/4)] \\
 N(S) &= S/\sinh(S) \\
 C_l^{m,n} &= \frac{4\pi}{2l+1} C_l Y_{lm}(\vec{h}) Y_{ln}(\vec{y}) \\
 C_l &= (2l+1)(\pi S/2)^{1/2} I_{l+1/2}(S)/\sinh S \\
 \mathcal{P}_{\vec{h}}(\vec{y}) &= N(S) I_0(S(1-z_1^2)^{1/2}(1-z_2^2)^{1/2}) \exp(Sz_1 z_2) \\
 z_1 &= (\vec{h}_i \cdot \vec{h}) \\
 z_2 &= (\vec{y} \cdot \vec{n})
 \end{aligned} \tag{4}$$

3. GAUSSIAN NORMAL DISTRIBUTION

Savjolova (1985) gave an expression for a distribution, that was derived from the central limit theorem of probability and gives a very common description of a texture component. All important terms are expressed through the series expansion coefficients C_l^{mn} , having the following form for the case of a canonical distribution (3 parameters α_{11} , α_{22} , α_{33}):

$$\begin{aligned}
 \|C_l^{mn}\| &= (2l+1) \exp(\|b_{mn}^l\|) \\
 b_{1+m,1+n}^l &= b_{2l+1-m,2l+1-m}^l = -\frac{1}{2}((2m+1)l - m^2)(\alpha_{11} + \alpha_{22}) - (l-m)^2 \alpha_{33} \\
 b_{1+m,3+m}^l &= b_{3+m,1+m}^l = b_{2l+1-m,2l-1-m}^l = b_{2l-1-m,2l+1-m}^l \\
 &= -\frac{1}{4}((m+1)(m+2)(2l-m)(2l-1-m))^{1/2}, \quad m = 0, 1, \dots, l \\
 \text{other } b_{ij} &= 0
 \end{aligned} \tag{5}$$

Although this function is of highest interest, its utilization for texture analysis meets serious complications, mainly due to the high computational effort: all characteristics are expressed in terms of series with coefficients given in form of a matrix exponentiation.

The special case of small halfwidths and a central distribution (5) revealed a very good agreement between (1) and (5), whereas (3) differs about 1% from (5) (Matthies, Muller, Vinel, 1988).

4. A NEW MODEL FUNCTION

4.1. ODF

The model function presented below was derived for use in a component analysis program, described by Helming, Eschner (1990), where the calculation of pole figure values is of main interest, so no expressions for C_l^{mn} will be given.

For this purpose Eq. (3) was modified: the halfwidth parameter S became directional dependent:

$$\begin{aligned} S &= \frac{1}{r^2} \\ \frac{1}{r^2} &= \frac{\vec{n}_x^2}{a^2} + \frac{\vec{n}_y^2}{b^2} + \frac{\vec{n}_z^2}{c^2} \\ \vec{n} &= g_d^{-1} \vec{n} \end{aligned} \quad (6)$$

with r taken from the $r(\vec{n})$ -representation of an ellipsoid (main axes a, b, c) and $\vec{n}$ taken from $gg_0^{-1} = [\omega, \vec{n}]$ (In some sense ω and $\vec{n}$ can be considered as functions of gg_0^{-1} , as will be done further on: $\omega = \omega(gg_0^{-1})$, $\vec{n} = \vec{n}(gg_0^{-1})$). g_d^{-1} rotates the ellipsoid out of it's trivial position.

Since

$$\begin{aligned} \forall g, g_d: g_d^{-1} \vec{n}(g) &= \vec{n}(g_d^{-1} g g_d) \\ \omega(g) &= \omega(g_d^{-1} g g_d) \end{aligned} \quad (7)$$

gg_0^{-1} can be substituted by $g_d^{-1} gg_0^{-1} g_d$ and the ellipsoid considered to be non-rotated.

With

$$A_{ii} = (1 - \cos \omega) n_i^2 + \cos \omega, \quad i = 1, \dots, 3 (x \dots y \text{ resp.}) \quad (8)$$

the diagonal matrix elements of $g_d^{-1} gg_0^{-1} g_d$ in it's $[\omega, \vec{n}]$ -representation and $A = 1/a$, $B = 1/b$, $C = 1/c$ we get:

$$\begin{aligned} -S(1 - \cos \omega) &= \alpha_0 + \alpha_1 A_{11} + \alpha_2 A_{22} + \alpha_3 A_{33} \\ \alpha_0 &= -\frac{1}{2}(A^2 + B^2 + C^2) \\ \alpha_1 &= \frac{1}{2}(-A^2 + B^2 + C^2) \\ \alpha_2 &= \frac{1}{2}(A^2 - B^2 + C^2) \\ \alpha_3 &= \frac{1}{2}(A^2 + B^2 - C^2) \end{aligned} \quad (9)$$

and finally (α_0 can be omitted due to the normalization)

$$\begin{aligned} f(g, g_d, g_0, A, B, C) &= N(A, B, C) \exp(-S(\vec{n})(1 - \cos \omega)) \\ &= N(A, B, C) \exp(\alpha_1 A_{11} + \alpha_2 A_{22} + \alpha_3 A_{33}) \\ \vec{n} &= \vec{n}(g_d^{-1} gg_0^{-1} g_d) \\ \omega &= \omega(g_d^{-1} gg_0^{-1} g_d) \\ |A_{ij}| &= g_d^{-1} gg_0^{-1} g_d \end{aligned} \quad (10)$$

4.2. Pole Figures

It is sufficient to give an expression for ideal pole figures (Matthies, Vinel, Helming, 1987):

$$\mathcal{P}_{\vec{h}}(\vec{y}) = \frac{1}{2\pi} \int_0^{2\pi} f(\{\vec{h}, \varphi\}^{-1}\{\vec{y}, 0\}) d\varphi \quad (11)$$

From (10) follows:

$$\begin{aligned} \mathcal{P}_{\vec{h}}(\vec{y}) &= \frac{N(A, B, C)}{2\pi} \int_0^{2\pi} \exp(\alpha_1 A_{11} + \alpha_2 A_{22} + \alpha_3 A_{33}) d\varphi \\ |A_{ij}| &= g^* \{\varphi\}^{-1} g^+ \\ g^* &= g_d^{-1} \{\vec{h}\}^{-1} = |A_{ij}^*| \\ g^+ &= \{\vec{y}\} g_0^{-1} g_d = |A_{ij}^+| \end{aligned} \quad (12)$$

With

$$\begin{aligned} x &= \alpha_1 A_{31}^+ A_{13}^* + \alpha_2 A_{32}^+ A_{23}^* + \alpha_3 A_{33}^+ A_{33}^* \\ y &= \alpha_1 (A_{11}^+ A_{11}^* + A_{21}^+ A_{12}^*) + \alpha_2 (A_{12}^+ A_{21}^* + A_{22}^+ A_{22}^*) \\ &\quad + \alpha_3 (A_{13}^+ A_{31}^* + A_{23}^+ A_{32}^*) \\ z &= \alpha_1 (A_{11}^+ A_{12}^* - A_{21}^+ A_{11}^*) + \alpha_2 (A_{12}^+ A_{22}^* - A_{22}^+ A_{21}^*) \\ &\quad + \alpha_3 (A_{13}^+ A_{32}^* - A_{23}^+ A_{31}^*) \end{aligned} \quad (13)$$

Eq. (12) becomes (see (19)):

$$\begin{aligned} \mathcal{P}_{\vec{h}}(\vec{y}) &= \frac{N(A, B, C)}{2\pi} \int_0^{2\pi} \exp(x + y \cos \varphi + z \sin \varphi) d\varphi \\ &= \frac{N(A, B, C)}{2\pi} \exp(x) \int_0^{2\pi} \exp(\sqrt{y^2 + z^2} \cos(\varphi - \bar{\varphi})) d\varphi \\ &= N(A, B, C) \exp(x) I_0(\sqrt{y^2 + z^2}) \end{aligned} \quad (14)$$

With the help of

$$\begin{aligned} g_d \vec{h} &= (h_x^*, h_y^*, h_z^*) \\ g_d^{-1} g_0 \vec{y} &= (y_x^+, y_y^+, y_z^+) \end{aligned} \quad (15)$$

Eqs. (13) and (14) can be rewritten as follows:

$$\begin{aligned} x &= \alpha_1 y_x^+ h_x^* + \alpha_2 y_y^+ h_y^* + \alpha_3 y_z^+ h_z^* \\ y^2 + z^2 &= x^2 + \alpha_1^2 (1 - y_x^{+2} - h_x^{*2}) \\ &\quad + \alpha_2^2 (1 - y_y^{+2} - h_y^{*2}) + \alpha_3^2 (1 - y_z^{+2} - h_z^{*2}) \\ &\quad + 2\alpha_1 \alpha_2 y_z^+ h_z^* + 2\alpha_1 \alpha_3 y_y^+ h_y^* + 2\alpha_2 \alpha_3 y_x^+ h_x^* \\ \mathcal{P}_{\vec{h}}(\vec{y}) &= N(A, B, C) \exp(x) I_0(\sqrt{y^2 + z^2}) \end{aligned} \quad (16)$$

4.3. Normalization

For both transformations $g^{(1)} = g_1 g$ and $g^{(2)} = g g_2$ the jacobians can be shown to equal 1:

$$\frac{\partial(a^{(1)}, \cos \beta^{(1)}, \gamma^{(1)})}{\partial(a, \cos \beta, \gamma)} = \frac{\partial(a^{(2)}, \cos \beta^{(2)}, \gamma^{(2)})}{\partial(a, \cos \beta, \gamma)} = 1 \quad (17)$$

Hence:

$$\forall g^{(1)}, g^{(2)}: \int f(g) dg = \int f(g^{(1)} g g^{(2)}) dg \quad (18)$$

when integration is performed over the whole Euler space. That means, for purposes of normalization g_d and g_o can be considered to be $\{0, 0, 0\}$.

With the help of

$$\frac{1}{\pi} \int_0^\pi \exp(x \cos t) \cos(nt) dt = I_n(x) \quad (19)$$

we obtain

$$\begin{aligned} N(A, B, C)^{-1} &= \frac{1}{8\pi^2} \int f(g) dg \\ &= \frac{1}{2} \int_{-1}^1 dt \exp(\alpha_3 t) I_0\left(\frac{A^2 - B^2}{2}(1-t)\right) I_0\left(\frac{C^2}{2}(1+t)\right) \end{aligned} \quad (20)$$

Probably, this expression cannot be simplified further. Nevertheless this rather simple term can easily be handled in numerical calculations.

5. EXAMPLES

Figure 1 shows a few special cases of the model distribution (16) including the case of central function and fibre (cubic/triclinic symmetry). For parameters see Table 1.

In pole figure 1, distribution (16) is shown for the case of $A = B = C$, when the ellipsoid of halfwidth parameters becomes a sphere and (16) identical to (3). A relation between the full width at half maximum b_{FWHM} and $A(B, C$ respectively) can be given:

$$\sqrt{A} = \ln(2)/[2 \sin^2(b_{FWHM}/4)] \quad (21)$$

Pole figures 2–4 illustrate the case of incomplete fibres with fibre axes in z - ($C < A = B$), x - ($A < B = C$) and y -direction ($B < A = C$), respectively.

Pole figure 5 shows a complete fibre with a fibre axis in x -direction ($A = 0$). This distribution is equivalent to (4). Equation (21) is valid, too.

In pole figure 6, a more common case of a distribution (16) is shown ($A \neq B \neq C, A \neq C$).

In Figure 2, X-ray pole figures of a Y-stabilized ZrO_2 -coating (obtained at DLR Köln by EB PVD) and recalculated pole figures from a single component texture model are compared. Model parameters can be found in Table 2.

The model reveals quantitatively a fibre direction ($\vartheta = 30.4^\circ$, $\varphi = 251.4^\circ$ in sample coordinate system) that was found to coincide with the direction of vapor deposition.

Figure 1 Example pole figures for special values of model parameters according to Table 1. Assumed crystal symmetry: cubic, sample symmetry: triclinic.

Table 1 Parameters of distributions shown in Figure 1, $g_d = \{0, 0, 0\}$, $g_0 = \{10^\circ, 10^\circ, 10^\circ\}$

Pole figure	1	2	3	4	5	6
(A, B, C)	(8, 8, 8)	(8, 8, 2.5)	(2.5, 8, 8)	(8, 2.5, 8)	(0, 8, 8)	(0, 2.5, 8)

Figure 2 Experimental and recalculated pole figures of a ZrO₂-coating. Component parameters can be found in Table 2.

Table 2 Parameters of the single component texture model of a ZrO₂-coating

	Intensity	Parameters
background	0.041	(A, B, C) = (8.096, 9.867, 3.146)
texture component	0.959	{ $\alpha_0, \beta_0, \gamma_0$ } = {113.5°, 1.74°, 0.86°}
		{ $\alpha_d, \beta_d, \gamma_d$ } = {251.4°, 30.4°, 349.6°}

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