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ANALYSIS OF THE ORIENTATION DIFFERENCE DISTRIBUTION FUNCTION IN THE TWO-PHASE MATERIAL USING MODEL FUNCTIONS

ANALIZA FUNKCJI ROZKŁADU RÓŻNIC ORIENTACJI W MATERIALE DWUFAZOWYM PRZY POMOCY FUNKCJI MODELOWYCH

Model representation of the texture in two-phase material was concerned in the paper. The orientation distribution function (ODF) can be interpreted as the superposition of Gauss-type distributions in the surroundings of preferred orientations. These model functions describe the main texture components with their parameters: volume fractions and scattering widths.

There exists a mathematical relation between the ODF and the orientation difference distribution function (ODDF). The ODDF can be analysed by relating its components and their parameters to the ODF component parameters. Such analysis of the ODDF demonstrates its statistical features, provided the ODF characteristics are known. Relations between ODF and the ODDF component parameters was determined and discussed in this work.

Keywords: texture, two-phase material, model orientation difference distribution function.

W pracy rozważano modelowe przedstawienie tekstury w materiale dwufazowym. Funkcja rozkładu orientacji (FRO) może być przedstawiona w postaci superpozycji rozkładów typu Gaussa wokół wyróżnionych orientacji. Takie modelowe funkcje opisują główne składowe tekstury przy pomocy parametrów, którymi są udziały objętościowe i szerokości rozmycia wokół wyróżnionych orientacji.

Pomiędzy FRO i funkcją rozkładu różnic orientacji (FRRO) istnieje matematyczna zależność. Na jej podstawie można analizować związek pomiędzy składowymi FRRO oraz FRO. Taka analiza - przy założeniu, że znana jest FRO – pozwala poznać właściwości FRRO. W pracy określono i przeanalizowano związek pomiędzy parametrami FRO i FRRO.

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1. Transformation of Orientation Distribution Function components into Orientation Difference Distribution Function

The orientation difference distribution function (ODDF) depends only on texture of material. The ODDF can be considered as a reference distribution function when grain boundaries have been characterized, in particular the crystallographic relations between grains. It concerns the all possible orientation relationships between grains in the material (ODDF is called the "uncorrelated" misorientation distribution [1, 2]) not only the relationships between neighbouring grains (the "correlated" misorientation distribution).

The ODDF analysis using its model representation is helpful for the better understanding the relationships between the orientation and the orientation difference distributions.

The orientation distribution function (ODF) in two-phase material — $f^{\alpha\beta}(g)$ consisting of α and β phases may be presented as the following sum:

$$f^{\alpha\beta}(g) = f^{\alpha}(g) + f^{\beta}(g), \tag{1}$$

with the conditions

$$\oint f^{\alpha\beta}(g) = 1, \oint f^{\alpha}(g) = V^{\alpha}, \oint f^{\beta}(g) = V^{\beta},$$

$$V^{\alpha} + V^{\beta} = 1,$$

where V^{α}, V^{β} represent the volume fractions of α and β phases.

The orientation difference distribution function (ODDF) — $f^{\alpha\beta}(\Delta g)$ corresponding with $f^{\alpha\beta}(g)$ is described by the following relation:

$$F(\Delta g) = \oint \left[\left(f^{\alpha}(g) + f^{\beta}(g)\right)\left(f^{\alpha}(\Delta g g) + f^{\beta}(\Delta g g)\right)\right] dg = \tag{2}$$

$$= F^{\alpha\alpha}(\Delta g) + F^{\beta\beta}(\Delta g) + F^{\alpha\beta}(\Delta g) + F^{\beta\alpha}(\Delta g),$$

$$F^{\alpha\alpha}(\Delta g) = \oint f^{\alpha}(g) f^{\alpha}(\Delta g g)\, dg$$

$$F^{\beta\beta}(\Delta g) = \oint f^{\beta}(g) f^{\beta}(\Delta g g)\, dg$$

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Let us assume that the functions f^α and f^β can be expressed as a superposition of Gaussian type distributions with the parameters $\left\{g_i^\alpha, V_i^\alpha, \Phi_i^\alpha; i = 1, I\right\}$ for phase α and $\left\{g_j^\beta, V_j^\beta, \Phi_j^\beta; j = 1, J\right\}$ for phase β, where $V_i^\alpha + V_j^\beta = 1$

$$f^\alpha(g) = \sum_{i=1}^{I} f_i^\alpha(g); \sum_{i=1}^{I} V_i^\alpha = V^\alpha \tag{3a}$$

$$f^\beta(g) = \sum_{j=1}^{J} f_j^\beta(g); \sum_{j=1}^{J} V_j^\beta = V^\beta. \tag{3b}$$

The components g_i and g_j defined by G a u s s i a n type distributions have the parameters $V_i^\alpha, \Phi_i^\alpha, V_j^\beta, \Phi_j^\beta$ representing volume fractions, and scattering widths around the positions g_i and g_j.

Such model distribution around position g_k may be represented by the equation [3]:

$$f_k(g) = H_k \exp\left(-\Phi^2/\Phi_k^2\right), \tag{4}$$

where

$$H_k = V_k 2\sqrt{\pi}\Big/\left\{\Phi_k\left[1 - \exp\left(\Phi_k^2/4\right)\right]\right\}$$

$$\Phi = \left|g \cdot g_k^{-1}\right|.$$

To carry out an analysis of the relationship between ODF and ODDF let us represent them as expansions into a series of generalised spherical functions ($T_l^{mn}(g)$) [3].

$$f(g) = \sum_{l,m,n} C_l^{mn} T_l^{mn}(g) \tag{5}$$

$$F(\Delta g) = \sum_{l,m_1,m_2} C_l^{m_1 m_2} T_l^{m_1 m_2}(\Delta g). \tag{6}$$

The coefficient of a series expansion of ODDF- $C_l^{m_1 m_2}$ and the coefficients of ODF - C_l^{mn} are connected by the relation [1]:

$$C_l^{m_1 m_2} = \frac{1}{2l+1} \sum_{n=-l}^{l} C_l^{m_1 n} C_l^{*m_2 n}. \tag{7}$$

For the function $F^{\alpha\alpha}, F^{\beta\beta}, F^{\alpha\beta}$ and $F^{\beta\alpha}$ we obtain respectively:

$$C_l^{m_1 m_2}(\alpha\alpha) = \frac{1}{2l+1} \sum_{n=-l}^{l} C_l^{m_1 n}(\alpha) C_l^{*m_2 n}(\alpha) \tag{8a}$$

$$C_l^{m_1m_2}(\beta\beta) = \frac{1}{2l+1}\sum_{n=-l}^{l} C_l^{m_1n}(\beta)\, C_l^{*m_2n}(\beta) \tag{8b}$$

$$C_l^{m_1m_2}(\beta\alpha) = \frac{1}{2l+1}\sum_{n=-l}^{l} C_l^{m_1n}(\beta)\, C_l^{*m_2n}(\alpha) \tag{8c}$$

$$C_l^{m_1m_2}(\alpha\beta) = \frac{1}{2l+1}\sum_{n=-l}^{l} C_l^{m_1n}(\alpha)\, C_l^{*m_2n}(\beta). \tag{8d}$$

If the orientation distribution around the position g_k is described by the relation (4), then we can consider approximately [4]:

$$C_l^{mn} \cong (2l+1)\sum_{i=1}^{I} \exp\left[-l\,(l+1)\,\frac{\Phi_i^2}{4}\right] V_i T_l^{*mn}(g_i). \tag{9}$$

Basing on the relation (8) and taking into consideration (9) we obtain the following expressions defining the coefficients of the series expansions of the functions $F^{\alpha\alpha}$, $F^{\beta\beta}$, $F^{\alpha\beta}$ and $F^{\beta\alpha}$:

$$C_l^{m_1m_2}(\alpha\alpha) = (2l+1)\sum_{i,i'}^{I} V_i^\alpha V_{i'}^\alpha \exp\left[-l(l+1)\frac{\left(\Phi_i^\alpha\right)^2+\left(\Phi_{i'}^\alpha\right)^2}{4}\right] T^{*m_2m_1}\left(\Delta g_{ii'}^\alpha\right) \tag{10a}$$

$$C_l^{m_1m_2}(\beta\beta) = (2l+1)\sum_{j,j'}^{J} V_j^\beta V_{j'}^\beta \exp\left[-l(l+1)\frac{\left(\Phi_j^\beta\right)^2+\left(\Phi_{j'}^\beta\right)^2}{4}\right] T^{*m_2m_1}\left(\Delta g_{jj'}^\beta\right) \tag{10b}$$

$$C_l^{m_1m_2}(\beta\alpha) = (2l+1)\sum_{i,j}^{I,J} V_i^\alpha V_j^\beta \exp\left[-l(l+1)\frac{\left(\Phi_i^\alpha\right)^2+\left(\Phi_j^\beta\right)^2}{4}\right] T^{*m_2m_1}\left(\Delta g_{ij}^{\alpha\beta}\right) \tag{10c}$$

$$C_l^{m_1m_2}(\alpha\beta) = (2l+1)\sum_{j,i'}^{J,I} V_j^\beta V_i^\alpha \exp\left[-l(l+1)\frac{\left(\Phi_j^\beta\right)^2+\left(\Phi_i^\alpha\right)^2}{4}\right] T^{*m_2m_1}\left(\Delta g_{ji}^{\beta\alpha}\right), \tag{10d}$$

$$\Delta g_{ii'}^\alpha = g_i^\alpha\left(g_{i'}^\alpha\right)^{-1}, \Delta g_{jj'}^\beta = g_j^\beta\left(g_{j'}^\beta\right)^{-1}, \Delta g_{ji}^{\beta\alpha} = g_j^\beta\left(g_i^\alpha\right)^{-1}, \Delta g_{ij}^{\alpha\beta} = g_i^\alpha\left(g_j^\beta\right)^{-1}$$

Hence, if the ODF components are described by $f^\alpha\left\{g_i^\alpha, V_i^\alpha, \Phi_i^\alpha; i = 1, I\right\}$ and $f^\beta\left\{g_j^\beta, V_j^\beta, \Phi_j^\beta; j = 1, J\right\}$, then the ODDF components have the following parameters:

$$\{\, \Delta g_{ii'}^{\alpha\alpha}, v_i^\alpha v_{i'}^\alpha, \sqrt{\left(\Phi_i^\alpha\right)^2+\left(\Phi_{i'}^\alpha\right)^2}; \Delta g_{jj'}^{\beta\beta}, v_j'^\beta v_{j'}^\beta, \sqrt{\left(\Phi_j^\beta\right)^2+\left(\Phi_{j'}^\beta\right)^2}; i, i' = 1, I, j, j' = 1, J \,\}$$

$$\{\, \Delta g_{ij}^{\alpha\beta}, v_i^\alpha v_j^\beta, \sqrt{\left(\Phi_i^\alpha\right)^2+\left(\Phi_j^\beta\right)^2}; \Delta g_{ji}^{\beta\alpha}, v_j^\beta v_j^\alpha, \sqrt{\left(\Phi_j^\beta\right)^2+\left(\Phi_i^\alpha\right)^2}; i = 1, I, j = 1, J \,\}.$$

2. Exemplary ODDF models

Example 1

Let us consider the simplest case for two components belonging to different phases g_1^α, g_1^β (Fig. 1):

Fig. 1. Scheme of the possible relations between two texture components: one in phase α and one in phase β

Let us assume that:

$$g_1^\alpha = \{107.5, 35.5, 111.5\}, V^\alpha = 0.7, \Phi^\alpha = 10°,$$

$$g_1^\beta = \{107, 26.5, 42\}, V^\beta = 0.3, \Phi^\beta = 5°,$$

where $g = \{\varphi_1, \Phi, \varphi_2\}, \varphi_1, \Phi, \varphi_2$ — Euler angles.

The corresponding differences of orientations may be defined with reference to the coordinates of the rotation axis (ϑ, ψ) and the angle of rotation ω about this axis

$$\Delta g_{ij}^{\alpha\beta} \equiv (\omega, \vartheta, \psi)$$
$$\Delta g_{11}^{\alpha\beta} = \{22, 24.3, 59.9\} \quad V^{\alpha\beta} = 0.21; \quad \phi = 11.18°$$
$$\Delta g_{11}^{\beta\alpha} = \{22, 24.3, 30.1\} \quad V^{\beta\alpha} = 0.21, \quad \phi = 11.18°$$
$$\Delta g_{11}^{\alpha\alpha} = \{0, 0, 0\} \quad V^{\alpha\alpha} = 0.49, \quad \phi = 14.14°$$
$$\Delta g_{11}^{\beta\beta} = \{0, 0, 0\} \quad V^{\beta\beta} = 0.09; \quad \phi = 7.07°.$$

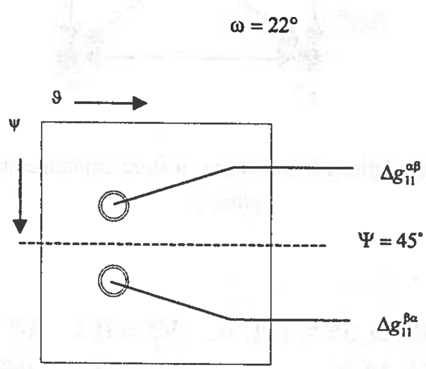

Fig. 2. Model ODDF

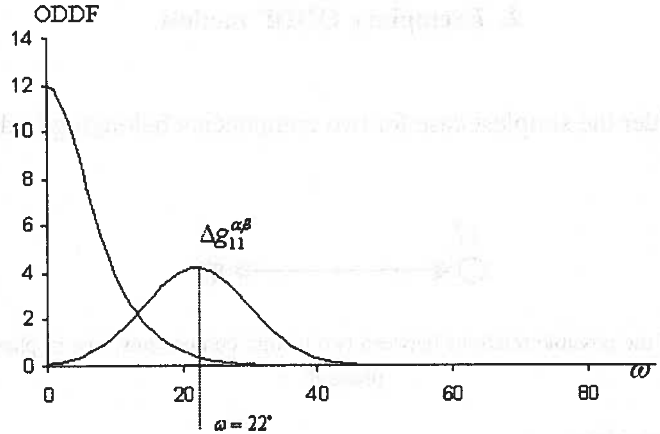

Fig. 3. ODDF profiles

The cross section ($\omega = 22°$)of the model ODDF is shown in Fig.2 and the ODDF intensity profiles in Fig.3:

Example 2

Let us now consider the case where the phases α and β consist of two components (Fig. 4):

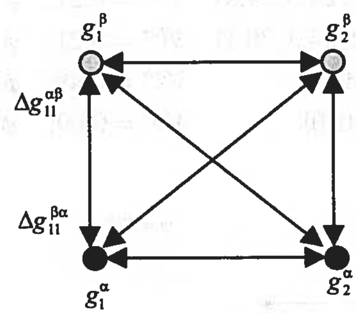

Fig. 4. Scheme of the possible relations between four texture components: two in phase α and two in phase β

$$
\begin{aligned}
g_1^\alpha &= (107.5, 35.5, 111.5), & V_1^\alpha &= 0.4, & \Phi_1^\alpha &= 10° \\
g_2^\alpha &= (55, 14, 0), & V_2^\alpha &= 0.2, & \Phi_2^\alpha &= 8° \\
g_1^\beta &= (107, 26.5, 42), & V_1^\beta &= 0.2, & \Phi_1^\beta &= 5° \\
g_2^\beta &= (62, 42, 12), & V_2^\beta &= 0.2, & \Phi_2^\beta &= 8°
\end{aligned}
$$

then the corresponding orientation differences are, as follows:

$$\Delta g_{11}^{\alpha\beta} = \{22, 24.3, 59.9\} V_{11}^{\alpha\beta} = 0.21, \phi = 11.18^\circ \quad \Delta g_{12}^{\alpha\alpha} = \{34.7, 34.1, 78.3\} V_{12}^{\alpha\alpha} = 0.12, \phi = 12.8^\circ$$

$$\Delta g_{11}^{\beta\alpha} = \{22, 24.3, 30.1\} V_{11}^{\beta\alpha} = 0.21, \phi = 11.18^\circ \quad \Delta g_{21}^{\alpha\alpha} = \{34.7, 34.1, 11.7\} V_{21}^{\alpha\alpha} = 0.12, \phi = 12.8^\circ$$

$$\Delta g_{12}^{\alpha\beta} = \{52.3, 34.2, 40.4\} V_{12}^{\alpha\beta} = 0.08, \phi = 12.8^\circ \quad \Delta g_{12}^{\beta\beta} = \{36, 53.3, 47.9\} V_{12}^{\beta\beta} = 0.06, \phi = 9.43^\circ$$

$$\Delta g_{21}^{\beta\alpha} = \{52.3, 34, 2, 49.6\} V_{21}^{\beta\alpha} = 0.08, \phi = 12.8^\circ \quad \Delta g_{21}^{\beta\beta} = \{36, 53.3, 42.1\} V_{21}^{\beta\beta} = 0.06, \phi = 9.43^\circ$$

$$\Delta g_{21}^{\alpha\beta} = \{20.9, 9.6, 66\}\, V_{21}^{\alpha\beta} = 0.09, \phi = 9.43^\circ \quad \Delta g_{11}^{\alpha\alpha} = \{0, 0, 0\}\, V_{11}^{\alpha\alpha} = 0.16; \phi = 14.14^\circ$$

$$\Delta g_{12}^{\beta\alpha} = \{20.9, 9.6, 24\}\, V_{12}^{\beta\alpha} = 0.09, \phi = 9.43^\circ \quad \Delta g_{11}^{\beta\beta} = \{0, 0, 0\}\, V_{11}^{\beta\beta} = 0.09; \phi = 7.07^\circ$$

$$\Delta g_{22}^{\alpha\beta} = \{33.5, 32.5, 88.8\}\, V_{22}^{\alpha\beta} = 0.6, \phi = 9.43^\circ \quad \Delta g_{22}^{\alpha\alpha} = \{0, 0, 0\}\, V_{22}^{\alpha\alpha} = 0.09; \phi = 11.31^\circ$$

$$\Delta g_{22}^{\beta\alpha} = \{33.5, 32.5, 1.2\}\, V_{22}^{\beta\alpha} = 0.6, \phi = 9.43^\circ \quad \Delta g_{22}^{\beta\alpha} = \{0, 0, 0\}\, V_{22}^{\beta\alpha} = 0.04; \phi = 11.31^\circ$$

The scheme of the ODDF in this case is shown in Fig.5 and the corresponding ODDF intensity profiles in Fig.6.

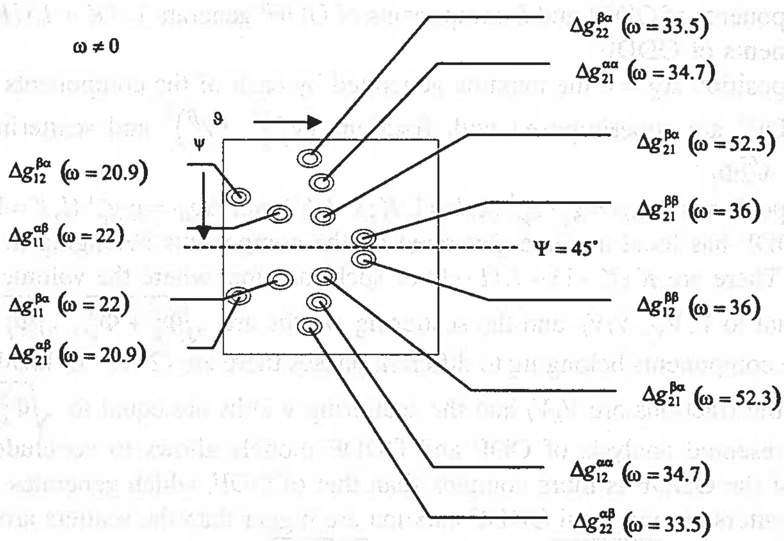

Fig. 5. Model ODDF

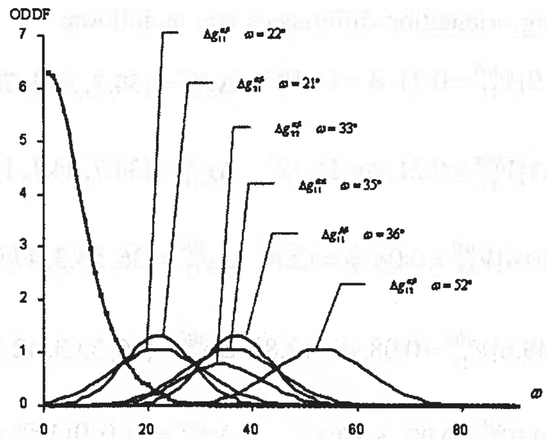

Fig. 6. ODDF profiles

3. Discussion and conclusions

Let us consider the case where ODF$^\alpha$ is composed of K components in the positions $\{g_k; k = 1, K\}$, the volume fractions V_k and the scattering widths Φ_k, while ODF$^\beta$ is composed of L components in the locations $\{g_l; l = 1, L\}$, the volume fractions V_l and the scattering widths Φ_l.

Analysis of equations (10) leads to the following conclusions as far as the ODDF is concerned:

- K components of ODF$^\alpha$ and L components of ODF$^\beta$ generate $1+(K+L)(K+L-1)$ components of ODDF.
- In the position $\Delta g = e$ the maxima generated by each of the components of ODF$^\alpha$ and ODF$^\beta$ are superimposed with fractions $\left(V_k^\alpha\right)^2$, $\left(V_l^\beta\right)^2$ and scattering widths $\sqrt{2}\Phi_k$, $\sqrt{2}\Phi_l$.
- In the positions $\Delta g_{kk'} = g_k \cdot g_{k'}^{-1}$ $(k, k = 1, K; k \neq k')$ and $\Delta g_{ll'} = g_l g_{l'}^{-1}$ $(l, l' = 1, L; l \neq l')$ the ODDF has local maxima generated by the components belonging to the same phase. There are $K(K-1) + L(L-1)$ of such maxima, where the volume fractions are equal to $V_k V_{k'}$, $V_l V_{l'}$ and the scattering widths are $\sqrt{\Phi_k^2 + \Phi_{k'}^2}$, $\sqrt{\Phi_l^2 + \Phi_{l'}^2}$.
- For the components belonging to different phases there are $(2 \cdot K \cdot L)$ local maxima, where the fractions are $V_k V_l$ and the scattering widths are equal to $\sqrt{\Phi_k^2 + \Phi_l^2}$.

The presented analysis of ODF and ODDF models allows to conclude that the structure of the ODDF is more complex than that of ODF, which generates it.

The scatters around local ODDF maxima are bigger than the scatters around ODF maxima $\left(\Phi_k \Phi_{k'} < \sqrt{\Phi_k^2 + \Phi_{k'}^2} \text{ and } \Phi_k \Phi_l < \sqrt{\Phi_k^2 + \Phi_l^2}\right)$ and the corresponding volume fractions are smaller: $\left(V_k^\alpha\right)^2$, $\left(V_l^\beta\right)^2$, $V_k V_l$.

REFERENCES

[1] H.J. Bunge, H. Weiland, Textures and Microstructures **7**, 231 (1988).

[2] F. Haeßner, K. Sztwiertnia, Proc. Eighth Int. Conf. on Textures of Materials ICOTOM-8, 1988 Santa Fe USA, Eds. J.S. Kallend, G.Gottstein, The Metallurgical Society, 163 (1988).

[3] H.J. Bunge, Texture Analysis in Material Science, Butterworths Publishers London (1982).

[4] J. Jura, J. Pospiech, G. Gottstein, Proc. Eleventh Int. Conf. on Textures of Materials ICOTOM-11, 1996 Xi'an China, Eds. Liang Z., Zuo L., Chu Y., Int. Academic Publishers, Beijing, China. **2**, 1351 (1996).

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