Simulation of complex magnesium alloy texture using the axial component fit method with central normal distributions

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Abstract. The component fit method in quantitative texture analysis assumes that the texture of the polycrystalline sample can be represented by a superposition of weighted standard distributions those are characterized by position in the orientation space, shape and sharpness of the scattering. The components of the peak and axial shapes are usually used. It is known that an axial texture develops in materials subjected to direct pressing. In this paper we considered the possibility of modelling a texture of a magnesium sample subjected to equal-channel angular pressing with axial components only. The results obtained make it possible to conclude that ECAP is also a process leading to the appearance of an axial texture in magnesium alloys.

1. Introduction

The subject of the study of quantitative texture analysis (QTA) is the experimental determination and interpretation of the statistical distribution of crystallites in polycrystalline materials. The knowledge of the preferential orientations of crystallites is necessary in particular to find out the influence of the technological process on the occurrence of preferential orientations [1]. The most commonly used in QTA values are functions describing crystallite distributions (ODF) and pole density functions - pole figures (PF) describing the distribution of crystallographic planes. ODF is defined on the rotation group of a three-dimensional space $SO(3)$ and pole figures are defined on a unit sphere $S^2$. The main problem of the QTA is simulation of an ODF $f(g)$ in a polycrystalline sample based on a set of experimentally obtained pole figures $\{P_{\hat{n}}(\hat{y})\}$. Among the various methods for solving this problem [1] - [5], the method of texture components [2] - [4], [6] has the advantage in the case of samples with low symmetry. Two types of components are usually considered. These are peak and axial ones. The first reaches its maximum at a certain point in the orientation space and has the form of a more or less wide bell. Averaging the peak component over all possible rotations about a fixed axis $\bar{n}$ generates an axial component that reaches a maximum on a certain circle in the rotation space.

2. The component fit method

The problem of an ODF simulation based on a set of pole figures is ill-posed because of the non-uniqueness of its solution [5] and the instability to measurement errors on pole figures [6]. The
uniqueness of the solution can be achieved on the class of functions that are the sum of fixed number of components with anchored positions in the orientation space. In our model, the ODF \( f(g), g \in SO(3) \) is represented by the sum of \( K \) texture components of with peak or axial scattering:

\[
f^\text{model}(g) = c_0 + \sum_{k=1}^{K} c_k f(g, g_{0k}, \vec{n}_k, \varepsilon_k),
\]

where \( c_k \) is the weight of corresponding component, \( g_{0k} \) is its maximum position, \( \vec{n}_k \) is an axis of axial component, \( \varepsilon_k \) is scattering parameter, \( c_0 \) is the volume fraction of the non-textured component. These parameters are to be determined. Considering the pole figures as integral projections of the ODF on the unit sphere:

\[
P_k(\vec{y}) = \frac{1}{4\pi} \int_0^{2\pi} f\left(\{\vec{h}, \phi\}^{-1}\{\vec{y}, 0\}\right) + f\left(\{-\vec{h}, \phi\}^{-1}\{\vec{y}, 0\}\right) d\phi,
\]

we get that any pole figure will be represented by the projections of the components of the PDF with the same parameters:

\[
P^\text{model}(\vec{h}, \vec{y}) = c_0 + \sum_{k=1}^{K} c_k P\left(\vec{h}, \vec{y}, g_{0k}, \vec{n}_k, \varepsilon_k\right),
\]

\( \vec{h}, \vec{y} \) are directions in the crystallite and the sample, respectively. We note that the normalization factors of the pole figures \( N_\lambda \) are also unknown parameters of the problem, since it is not possible to normalize pole figures in the process of measurement because of incompleteness of the data. In this work unknown model parameters are searched by minimizing the square of the weighted residual taken at all measured points on all pole figures:

\[
r^2 = \sum_{\lambda=1}^{N} \sum_{i=1}^{f} \sum_{j=1}^{j} W(\lambda, i, j) \left| N_\lambda P_{h_i}(\vec{y}_j) - P^\text{model}(\vec{h}_i, \vec{y}_j) \right|^2 \rightarrow \min.
\]

This problem of non-linear optimization is solved numerically. To achieve the stability of the solution, regularization is applied [7] - [9]. The desired ODF is constructed from the received parameters of the model. The adequacy of the model is estimated using the \( RP \)-value:

\[
RP(\Delta) = \frac{1}{N(\Delta)} \sum_{\vec{y} \in \gamma} \left| \frac{P_{h_\gamma}(\vec{y}) - P^\text{model}(\vec{h}_\gamma, \vec{y})}{P_{h_\gamma}(\vec{y})} \right| \cdot 100\%,
\]

where the summation is carried out over all points at which the experimentally measured magnitude of the pole density is not less than the parameter \( \Delta \), and \( N(\Delta) \) is the number of these points [1], [6].

### 3. Simulation of complex magnesium alloy texture

We consider a sample of magnesium alloy Mg-4.5% Nd subjected to equal-channel angular pressing (ECAP). The crystal lattice of magnesium has a hexagonal symmetry. The symmetry of the sample is monoclinic. The presence of a low symmetry determined the choice of component fit method for the ODF simulation. For this sample, six incomplete non-normalized pole figures were obtained by X-ray diffraction. There were visually determined individual maxima and rings of increased pole density on experimental pole figures. The individual maxima were supposed to be modeled by peak components. However, no reasonable number of peak components made it possible to adequately describe the available PFs, therefore, the possibility of pole density approximation by superposition of only the axial components was considered. It turned out that with a certain overlapping of each other, the axial components also create peaks of pole density of the type, as in the available experimental PFs. In the process of approximation it is established that all pole figures can be adequately described by a model including seven axial components and a background component. Figure 1 shows the positions of the axial components on the stereographic projections of pole figures [10-13], [10-11], [10-10].
Figure 1. The positions of the seven axial texture components of the magnesium sample on the pole figures [10-13], [10-11], [10-10] are listed in descending order of the component weights.
The components found have the following parameters:

\[ c_1 = 29.8, \quad \epsilon_1 = 0.010, \quad \bar{n}_1 = \left\{ 259.2^\circ, 23.0^\circ \right\}, \quad g_{01} = \left\{ 259.2^\circ, 23.9^\circ, 9.9^\circ \right\}, \]
\[ c_2 = 18.7, \quad \epsilon_2 = 0.012, \quad \bar{n}_2 = \left\{ 295.2^\circ, 30.1^\circ \right\}, \quad g_{02} = \left\{ 295.2^\circ, 32.3^\circ, 14.9^\circ \right\}, \]
\[ c_3 = 13.3, \quad \epsilon_3 = 0.007, \quad \bar{n}_3 = \left\{ 223.2^\circ, 32.6^\circ \right\}, \quad g_{03} = \left\{ 223.2^\circ, 39.5^\circ, 14.9^\circ \right\}, \]
\[ c_4 = 8.7, \quad \epsilon_4 = 0.024, \quad \bar{n}_4 = \left\{ 259.2^\circ, 43.7^\circ \right\}, \quad g_{04} = \left\{ 79.2^\circ, 37.0^\circ, 9.8^\circ \right\}, \]
\[ c_5 = 6.3, \quad \epsilon_5 = 0.014, \quad \bar{n}_5 = \left\{ 74.7^\circ, 36.5^\circ \right\}, \quad g_{05} = \left\{ 74.7^\circ, 43.4^\circ, 14.9^\circ \right\}, \]
\[ c_6 = 4.9, \quad \epsilon_6 = 0.010, \quad \bar{n}_6 = \left\{ 114.3^\circ, 37.3^\circ \right\}, \quad g_{06} = \left\{ 114.3^\circ, 44.3^\circ, 14.9^\circ \right\}, \]
\[ c_7 = 3.4, \quad \epsilon_7 = 0.008, \quad \bar{n}_7 = \left\{ 90.0^\circ, 32.7^\circ \right\}, \quad g_{07} = \left\{ 90.0^\circ, 35.9^\circ, 14.9^\circ \right\}, \quad c_0 = 14.9. \]

For the model found we obtain the values \( RP(0.5) \approx 14\% \), \( RP(1.0) \approx 10\% \). Figure 2. shows the experimental and model pole figures [0004] and [10-11] in the form of the level lines of the pole density on stereographic projections.

![Figure 2](image2.png)

**Figure 2.** Experimental and model pole figures [0004] and [10-11].

![Figure 3](image3.png)

**Figure 3.** The isolines of the orientation distribution function at zero section.

The model ODF with axial components with central normal distribution (Legendre polynomials) is constructed on the basis of the parameters found:

\[ f(g) = c_0 + \sum_{k=1}^{7} c_k \sum_{l=0}^{\infty} (2l + 1) \exp(-l(l+1)\varepsilon_k^2) P_l(g\bar{n}_k, g_{0k}\bar{n}_k). \]

The ODF isolines for the sample of the magnesium alloy at zero section are shown in figure 3.

**4. Conclusion**

It is shown that texture development of magnesium alloys in the process of equal-channel angular pressing proceeds according to the principle of axial components formation. The complex magnesium alloy Mg-4.5% Nd texture in the sample subjected to ECAP can be adequately described by a superposition of seven axial components with a central normal distribution.
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