Comparison of the model EBSD experiment results with the PF and ODF obtained experimentally

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Abstract. For study of EBSD parameters impact on the evaluation of the polycrystalline texture characteristics the mathematical model of EBSD experiment was developed. The specimen and experiment simulation allows us to compare texture entities calculated directly from specimen with corresponding ones obtained from model measurements. By the EBSD parameters a scanning step and a threshold disorientation angle are meant. In the given work the comparison of Pole Figures and Orientation Distribution Function calculated from model EBSD measurements and corresponding entities, obtained from real EBSD data, is presented. The most significant results are formulated.

1. Introduction

The problem of choosing measurement parameters in electron back scattering diffraction (EBSD) [1] remains insufficiently investigated, while these parameters have a large effect on measurement results. It was indicated than an unsuitable choice of measurement parameters leads to incorrect results. For example, an insufficient number of orientation measurements results in low accuracy of computed Pole Figures (PFs) [2]; disorientation angle measurements may lead to inconsistent average grain size values [3]; a small step of measurements leads to a considerable increase in time required for conducting an experiment (see [4]). To study the problem of EBSD parameters choosing we need the opportunity to compare the specimen data and obtained EBSD data. Accordingly, it is of interest to study this issue with the help of the mathematical simulation of an experiment.

Below we develop a two-dimensional mathematical model of a specimen and a subsequent EBSD experiment conducted for various sets of EBSD parameters. To study the impact of the measurement parameters PF and Orientation Distribution Function (ODF) of a model specimen and corresponding ones, calculated from model EBSD measurements, are compared. The real EBSD experiment was also performed. The results of the model experiment are correlated with such detected in the real EBSD data.

2. Specimen and experiment simulation

A specimen is a set of grains

\[ \{ (x_i, g_i, \omega_i) \ i = 1, 2, \ldots, N - 1, (x_N, g_N) \} \]  

(1.1)
where \( x_i \) is the size of the \( i \)th grain, which is equal to the diameter of a circle whose area is equal to that of the grain’s cross section; \( g_t = (\phi_t, \theta_t, \psi_t) \) is the orientation of the \( i \)th grain corresponding to the Euler angles \(-\pi \leq \phi_t, \psi_t \leq \pi, 0 \leq \theta_t \leq \pi; \omega_i = (g_i, g_{i+1}) \) is the disorientation angle between neighboring grains; and \( N \) is the number of grains in the specimen. Grain sizes are modeled by Neumann’s method as random variables distributed satisfying a gamma distribution [5].

A set of grain orientations is generated by the special Monte-Carlo method with a distribution function in the form of central distribution function (CND) [6] with a given parameter \( \varepsilon > 0 \). Grains in equation (1.1) are separated by boundaries, which are variables uniformly distributed in \([0, 2\gamma/10]\), where \( \gamma > 0 \) is such that the area of the boundaries is 10% of the grains’ area.

To simulate the EBSD experiment the following measurement parameters are specified: \( h \) is the scanning step, and \( \omega_0 \) is a threshold disorientation angle for determining two different neighboring grains \( g_i \) and \( g_{i+1} \) from the disorientation angle between them.

Measurements are made at the lattice points \( \Delta_k = kh, k = 1, 2, ..., N_1 \) on the surface of the simulated specimen. If the point hits the boundary, it is assigned an orientation corresponding to the Euler angles equal to the arithmetic mean of the angles of two nearest determined orientations [6]. The resulting orientations are used to calculate the disorientation angles \( \tilde{\omega}_k = (\hat{\varphi}_k, \hat{\psi}_k) \), \( k = 1, ..., N_1 - 1 \). If \( \tilde{\omega}_k \leq \omega_0 \), then the \( 4 \)th and \((k + 1)\)th steps belong to a single grain. If \( n \) measurements are inside the \( j \)th grain, then the grain size is set equal to \( x_j = nh \) and the Euler angles are calculated as the arithmetic mean of the corresponding \( n \) measurements. If \( \tilde{\omega}_k > \omega_0 \), then a new grain begins at the point \((k + 1)h\). As a result of the measurements, we obtain a set of grains

\[
\{(\tilde{x}_i, \tilde{g}_i, \tilde{\omega}_i), i = 1, 2, ..., N_1 - 1, (\tilde{x}_N, \tilde{g}_N)\}. \tag{1.2}
\]

For calculation of ODF the following kernel ODF estimator for a sample of orientations in equations (1.1) and (1.2) was used

\[
f_N(g) = \frac{1}{(\alpha)^3} \sum_{i=1}^{N} C_i q_1 \left( \frac{\varphi - \phi_i}{\alpha} \right) q_3 \left( \frac{\psi - \psi_i}{\alpha} \right) q_2 \left( \frac{\cos \theta - \cos \theta_i}{\alpha} \right), C_i = \frac{x_i}{\sum_{i=1}^{N} x_i}; \tag{1.3}
\]

where \( q_i(t), i = 1, 2, 3 \) are are smoothing kernels (see [6]).

A statistical estimate of PF with a kernel in the form of CND has the form [7]

\[
P_\alpha(y) = \sum_{l(2)=0}^{\infty} (2l + 1) \exp(-l(l + 1)\alpha^2) \sum_{i=1}^{N} C_i P_l^4 (g_{\tilde{y}}^{-1}g_{\tilde{h}}^{-1}g_{h}(3,3)), C_i = \frac{x_i}{\sum_{i=1}^{N} x_i}; \tag{1.4}
\]

where \( \alpha \) is the kernel smoothing parameter (playing the role of regularisation parameter); \( P_l^4 \) are Legendre polynomials; \( g_{\tilde{y}}^{-1}g_{\tilde{h}}^{-1}g_{h}(3,3) \) is the element with index \( 3 \times 3 \) of the rotation matrix \( g_{\tilde{y}}^{-1}g_{\tilde{h}}^{-1}g_{h}, g_{\tilde{y}} = \{\tilde{y}, 0\}, g_{\tilde{h}} = \{\tilde{h}, 0\} \).

3. Comparison of the results for model and real experiments

In the real EBSD experiment material for the investigation was a ferritic-martensitic steel EP823 (12Cr-Mo-W-Si-V-Nb-B) treated by the nitrogen gas high-temperature pulsed plasma flows (HTPPF). HTPPF surface modification were carried out by means of the Z-pinch type experimental plasma installation “Desna-M” [8]. This treatment results in the formation of the microcrystalline surface layer with a mean grain size of 2 mm. This layer has a single phase bcc type (a-Fe) equiaxed grain structure with a homogeneous distribution of alloying elements. An EBSD data were acquired using the HKL CHANNELS software (Oxford Instruments, UK) coupled to an EVO 50 XVP scanning electron microscope (ZEISS, Germany). EBSD measurement were performed with scanning step sizes \( h = \).
0.5 μm, 1.0 μm, 2.0 μm and then for each step size meaning the different threshold disorientation angle meanings were considered: \( \omega_0 = 5^\circ, 10^\circ \) and \( 20^\circ \).

Following the scheme described in Section 2, we modeled specimen, which is similar in the main properties with the sample in the real experiment. It is single-phased material with average grain size equal to 2.0 μm. As the grain orientations were modeled by the special Monte-Carlo method for CND on \( SO(3) \), shown in equation (1.2), with texture sharpness \( \varepsilon = 1/8 \) (see [6]), the simulated sample has strong texture. The number \( N \) of grains in a specimen was set equal to 1000. The following EBSD measurement parameters were chosen for model measurements: \( h = 0.5 \, \mu m, 1.0 \, \mu m, 2.0 \, \mu m \); \( \omega_0 = 5^\circ, 10^\circ \) and \( 20^\circ \). Below, the results of observations concerning the ODF and PF changing according to EBSD measurement parameters are given.

3.1. Influence of the EBSD parameters on PFs calculation

According to the results of specimen PF and PF of model measurements comparing it was obtained that for strongly textured specimens threshold disorientation angle is appeared to be more significant than scanning step; for weakly textured specimens, conversely, measurements are strongly affected by the scanning step [9]. The calculated RP-factor for measured PF, imaged on figure 1, verifies statement mentioned.

![Figure 1](image)

**Figure 1.** Dependences of the RP factor of the pole figures on the threshold misorientation angle.

There for calculation of the RP-factor the following formula is used

\[
RP = \frac{1}{I} \sum_{i,j=1}^{n_i,n_j} \left| \frac{\hat{P}_N(\eta_i, \chi_j) - \hat{P}_N(\eta_i, \chi_j)}{\hat{P}_N(\eta_i, \chi_j)} \right| \cdot 100\%,
\]

(2.1)

where \( \hat{P}_N(\eta, \chi) \) is a kernel estimate of PF for the model specimen, \( \hat{P}_N(\eta, \chi) \) is a kernel estimate of PF for result of measurements of the model specimen, \( I \) is a total number of partition cells.

According to the results of the real EBSD experiment PFs are strongly affected by the threshold disorientation angle (see figure 2), the influence of step size on PF evaluation is not so significant (see figure 3). The given statement is in a good agreement with the model experiment results.
Figure 2. PF for fixed $h = 0.5 \mu m$, (a) for $\omega_0 = 5^\circ$ and (b) for $\omega_0 = 20^\circ$.

Figure 3 showes that PF for essentially different step sizes $2.0 \mu m$ and $0.5 \mu m$ the quite similar results were obtained.

Figure 3. PF for fixed $\omega_0 = 10^\circ$, (a) for $h = 2.0 \mu m$ and (b) for $h = 0.5 \mu m$. 
It is worth to mention that at that the time expended in EBSD measurement for step sizes 2.0μm and 0.5μm increases by a factor of several tens under step size growth (from 10 minutes up to 2 hours 34 minutes).

We should also notice that according the results of simulation the PF maximum and its position are unstable to EBSD measurements parameters. Instability grows with weakening of specimen texture sharpness. It shows up in the shift of PF maximum position or second maximum appearing. The more grain size distribution approaches the uniform one, the stronger instability and the less accurate PF calculation [9].

In the real experiment the behavior of PF maximums was also considered. Table 2 presents PF maximums according to different EBSD parameters.

| h (μm) | ω₀ (°) | 20° | 10° | 5° |
|-------|--------|-----|-----|-----|
| 2.0   | 5.56   | 4.85| 4.82|
| 1.0   | 4.93   | 4.11| 4.23|
| 0.5   | 4.85   | 4.02| 4.15|

Let us notice that PF maximum increases under step size growth for each fixed ω₀, but dependence of the PF maximum on the threshold disorientation angle is appeared to be not so clear: the maximum can increase or decrease with ω₀ growth. Such a behavior points out an instability of the PF calculation to EBSD parameters that is obtained in the model experiment mentioned above.

3.2. Influence of the EBSD parameters on ODF calculation

Below, the comparison of the ODF obtained from EBSD orientation data with ones calculated in the simulated experiment according to EBSD measurement parameters are given.

As well as for PFs the impact of a scanning step is appeared to be not such significant for ODF recovering from individual orientations. At the same time, the statistical sample is reduced substantially. For more detail on the effect of a sample on ODFs recovered from individual orientations, see [10].

At the same time in both experiments it was found out that ODF is also strongly affected by the threshold disorientation angle. For ODF at ω₀ = 20° and, in some cases, for ω₀ = 10°, the maximum is observed to increase [5]. This behavior of the ODF is similar to that in the presence of dependent orientations [6], when the ODF maximums arise at ω₀ = 20° because of merging a large number of grains. What about the coordinates of the maximum we can not reasonably confirm whether they remain unchanged or not while the variable ψ is fixed. In the cased of strongly textured specimens, the ODF should be recovered with a small threshold disorientation angle. For the specimens under consideration, as such an angle, we can use ω₀ = 5°.

Relying on the contour lines of ODF cross section (see figure 4) we receive the sufficient maximums growing (almost twice) for ω₀ = 20° versus ones for ω₀ = 5° and 10°. Angles φ1, Φ, φ2 on figure 4 correspond to Euler angles φ, θ, ψ respectively. Besides unsuitable meaning of ω₀ may changed ODF character. This observation was also found out during the processing of model experiment results [5].
Figure 4. Contour lines of ODF cross section for fixed $h = 0.5 \, \mu m$, (a) for $\omega_0 = 20^\circ$ and (b) for $\omega_0 = 10^\circ$.

4. Conclusions

The processing of the model and real experiments observations has pointed out the correlation between behavior of texture entities obtained from simulated and really performed experiments. This fact gives us the ability to use our model for study of choosing measurement parameters. For strong textured material a step size changing does not lead to substantial changing in PFs and ODF calculation. The step size being less than a quarter of average grain size can result in unjustifiably high time of measuring in view of inessential result improvement. Thus, for the single-phase strong textured specimen with small amount of boundaries the threshold disorientation angle should not be more than 10° and the step size equal to half an average grain size is suitable.

To choose parameters for measurement of a specimen with other properties the corresponding modeling with new characteristics and further model experiment with parameters varying are needed to be conducted.

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