A novel approach of the grain structure modelling in the framework of polycrystalline specimen and EBSD experiment simulation

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Abstract. In this work the influence of the grain structure model in polycrystalline specimen on the results of the simulated EBSD experiment is studied. In the framework of EBSD experiment simulation the improved model of the polycrystalline with the grains in form of ellipses is used. Such a model is proposed to describe structural features of the real specimen more elaborately than one with grains as circles. Matching the improved polycrystalline model with the initial one is performed by comparison of the texture entities, restored from the EBSD measurements of specimens, with reference ones, calculated for modelled specimens. The EBSD experiment simulation is conducted for both specimens models under varying of the experiment parameters: a scanning step and a tolerance angle.

1. Introduction
The EBSD (Electron Back Scattering Diffraction) experiment parameters influence study, a scanning step and a tolerance angle, on the reliability of the obtained results of the EBSD experiment is proved to be of crucial importance [1, 2]. Experimental nature of material investigations by means of EBSD does not allow to compare the experiment results with the original specimen characteristics to tune the parameters of measurements [3]. The specimen and experiment simulation makes it possible to compare texture entities calculated directly from specimen with corresponding ones obtained from simulated EBSD measurements.

In this work the attempt to improve the model of EBSD experiment proposed earlier in [4, 5] was performed by utilizing the novel approach for grain structure modelling in the framework of polycrystalline model. In the advanced grain structure model grains were considered in the form of rotated ellipses instead of circles used in [4, 5]. The proposed model of the grain structure is based on specificity of the EBSD measurements processing, as in the commercial software [6] the plane cross sections of grains are approximated by ellipses (figure 1). Matching the improved polycrystalline model with the initial one was performed by comparison of the texture characteristics, calculated from the EBSD measurements, conducted for both models under varying of the experiment parameters: scanning step and tolerance angle. As texture characteristics orientation distribution function (ODF) [7], disorientation density distribution function (DDDF) and texture index (TI) were considered [8]. The dependence of TI on the experiment parameters, calculated for simulated measurements of specimens with both grain structure models, was compared with one, calculated for ferritic-martensitic steel EP823 [9].
2. Methods

2.1. Description of the polycrystalline specimen and EBSD experiment models

A model specimen was considered as a statistical object. Two distinct model specimens $\bar{S}_{\text{cir}}$ and $\bar{S}_{\text{ell}}$ consisting of $N = 1000$ grains were created:

$$
\bar{S}_{\text{cir}} = \{ \bar{U}_{\text{cir}}, i = 1, ..., N \}, \bar{U}_{\text{cir}} = [x, \omega, g(\varphi, \theta, \psi), \delta],
$$

(1)

$$
\bar{S}_{\text{ell}} = \{ \bar{U}_{\text{ell}}, i = 1, ..., N \}, \bar{U}_{\text{ell}} = [x, c, \omega, g(\varphi, \theta, \psi), \delta].
$$

(2)

The vectors $\bar{U}_{\text{cir}}$ and $\bar{U}_{\text{ell}}$ so defined were proposed to be the grain models. In $\bar{U}_{\text{cir}}$, the grains' cross sections were modelled as circles sequentially located and $x$ was proposed to be the size of the grain determined as a diameter of a corresponding circle (figure 2 (a)). In the improved specimen model the grains' cross section was considered as ellipse with grain size $x$, also calculated as a diameter of circle equal to the grain’s cross section with respect to its area, but the following EBSD measurements were performed along chords $c$ of ellipse approximating the plane cross section of the grain (figure 2 (b,c)). Grain sizes $x$ were modelled by Neumann's method as random variables distributed satisfying a gamma distribution $\Gamma(2,1)$ so that the mean grain size $\bar{x}$ was equal to 2.0 $\mu$m [4, 5].

A grain boundary between the given grain and the following one $\delta$ was a variable uniformly distributed in $[0, 2\bar{x}/10]$, so that the total size of the boundaries is 10% of the grains’ total size.

![Figure 1](image1.png)  
**Figure 1.** The EBSD map of the steel specimen, where grains' cross sections are approximated by ellipses

![Figure 2](image2.png)  
**Figure 2.** Schemes of the model specimens (a,b) and the individual grain in form of ellipse (c)

For both specimens the same orientations sample was utilized (equal grain orientations are shown on figure 2 (a,b) by the same color of the circle and the corresponding ellipse), orientations $g(\varphi, \theta, \psi)$ were modelled by Monte-Carlo method with ODF in the form of central normal distribution (CND) [7, 10]:

$$
\text{CND}(\mu, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}
$$

where $\mu$ is the mean value and $\sigma$ is the standard deviation.
\[
f(t)dt = \sum_{l=0}^{\infty} (2l+1) \exp \left\{ -l(l+1)\varepsilon^2 \right\} \chi_l \frac{1}{\pi} \sin^2 \frac{t}{2} dt,
\]

where \( t \in [-\pi; \pi] \), \( \cos \frac{t}{2} = \cos \frac{\phi+\psi}{2} \cos \frac{\theta}{2} \), \( \chi_l = \sin \left( \frac{l+1}{2} \right) / \sin \frac{t}{2} \) are the characters of the rotation group SO(3) representation; \( \frac{1}{\pi} \sin^2 \frac{t}{2} dt \) – invariant measure, \( \varepsilon = 1/8 \) – texture sharpness.

\( \omega \) in equations (1), (2) denotes a disorientation angle between two neighboring grains [7].

Thus, the specimens \( \mathcal{S}_{cir} \) and \( \mathcal{S}_{ell} \) had equal texture characteristics and equal mean grain size 2.0 \( \mu m \), but different grain structure (rotated ellipses and circles, as shown on figure 2 (a,b)).

Let us define an operator \( \Phi(\mathcal{S}, h, \omega_0) \), modelling the result of EBSD study of the specimen \( \mathcal{S} \) under the parameters \( (h, \omega_0) \), where \( h \in (0, H), H > 0 \) – scanning step over the modelled surface of specimen, \( \omega_0 \in \Omega_0 \subseteq (0, \pi) \) – tolerance angle. We assumed, that for \( \mathcal{S}_{cir} \) the measurements are made along circles diameters, whereas for specimen \( \mathcal{S}_{ell} \) orientation scanning was performed along the ellipses chords. A chord of ellipse can be calculated as

\[
c = \frac{x}{\sqrt{(\cos \alpha)^2/k + k(\sin \alpha)^2}}
\]

where \( x \) is the diameter of the circle with equal area, \( \alpha \) – an angle of the ellipse rotation, \( k = a/b \) (see figure 2 (c)). The proposed ellipse approach seemed to be more reliable according to a procedure of the real EBSD experiment (figure 1).

The results of simulated EBSD measurements of both specimens \( \mathcal{S}_{cir} \) and \( \mathcal{S}_{ell} \) can be presented as

\[
\mathcal{S}_{cir} = \left\{ \mathbf{r}_{cir,i}, i = 1, ..., \tilde{N} \right\}, \quad \mathbf{r}_{cir} = \left[ \mathbf{x}_{cir}, \mathbf{g}(\phi, \theta, \psi) \right],
\]

\[
\mathcal{S}_{ell} = \left\{ \mathbf{r}_{ell,i}, i = 1, ..., \tilde{N} \right\}, \quad \mathbf{r}_{ell} = \left[ \mathbf{x}_{ell}, \mathbf{g}(\phi, \theta, \psi) \right].
\]

As it can be seen from equations (5), (6) different approaches of specimen modelling result in the difference of simulated measurements procedure, causing the change of all grain properties, restored from measurements.

2.2. Texture characteristics for verification of the novel grain structure model

To compare considered grain structure models the behaviour of texture characteristics: ODF, DDDF, TI, – under varying the parameters \( (h, \omega_0) \) was investigated. For calculation of ODF and TI from the set of individual orientations the kernel estimation method was used:

\[
f_N(t) = \frac{1}{\alpha} \sum_{i=1}^{N} C_i q \left( \frac{t - t_i}{\alpha} \right), \quad C_i = \frac{x_i}{\sum_{i=1}^{N} x_i}, \quad t \in [-\pi; \pi], \quad \cos \frac{t}{2} = \cos \frac{\phi + \psi}{2} \cos \frac{\theta}{2}.
\]

where \( q(t) \) is a Gaussian kernel, \( \alpha \) – smoothing parameter.

For calculation of TI for ODF in form of CND (equation 3) the following estimate was used [7]:

\[
J_{mod} = \sum_{l=0}^{K} |\mathbf{c}_l|^2, \quad \mathbf{c}_l = \frac{1}{N} \sum_{i=1}^{N} \sin \left( \frac{l+1}{2} \right) t_i \sin \frac{t_i}{2}, \quad \beta \in [-\pi; \pi], \quad \cos \frac{t}{2} = \cos \frac{\phi + \psi}{2} \cos \frac{\theta}{2}.
\]
To compare the reference ODF and DDDF of the model specimens with corresponding ones, restored from EBSD measurements, chi-square homogeneity test was used [11].

3. Results

3.1. Comparison the circle and ellipse grains structure models with respect to the texture characteristic restored from the corresponding simulated EBSD measurements

For model specimens described by equations (1), (2) the simulation of EBSD experiment results was performed for the given set of parameters meanings [4, 5]: $h = 0.5 \, \mu m; 1.0 \, \mu m; 2.0 \, \mu m; \omega_0 = 5^\circ, 10^\circ, 20^\circ$. The application of two distinct approach for specimen modelling led to quite similar results of all texture characteristics restored from the simulated EBSD data of corresponding specimens.

DDDF and ODF were appeared to be effected by tolerance angle stronger than scanning step for both modelled specimens. This was in agreement with the chi-square homogeneity test, showing that the hypothesis on the coincidence of the DDDF of each specimen and corresponding measurements was accepted at 95% confidence level only for small $\omega_0 = 5^\circ$ and for the steps $h = 2.0, 1.0 \, \mu m$. Figure 3 represents DDDF histograms for two parameters sets when tested hypothesis was accepted (figure 3 (a)) and declined (figure 3 (b)).

For both grain structure models ODF showed close behaviour under parameters varying. The hypothesis on the coincidence of the one-parameter ODFs (equation (7)) was rejected at $\omega_0 = 20^\circ$. In this case, the ODFs, restored from modelled measurements, oscillate on the “tails” and the central minimum decrease. In the other cases of parameters sets, it was accepted at 95% confidence level.

![Figure 3](image)

**Figure 3.** DDDF histograms for specimen (spec), EBSD measurements of specimen with grains as circles (meas_cir) and for corresponding ones of specimen with grains as ellipses (meas_ell), (a) the hypothesis on the coincidence of the DDDF of each specimen and corresponding measurements is accepted, (b) – rejected. The vertical lines: dotted, dashed, dash-dotted, – correspond to mean values of the specimen, meas_ell, meas_cir disorientation angles, respectively.
3.2. Results of the TI calculation from the modelled EBSD data of specimens with two distinct grain structure. Comparison TI of the simulated EBSD measurements with one of the steel EP823

The TI is a measure of texture severity: tending of TI to unit points out weak texture of specimen, for the case of strong texture TI shows infinite increase[1, 8, 12].

The TI calculation from the EBSD measurements demonstrated slightly different results for both modelled specimens. The dependence of the TI relative error on the experiment parameters \((h, \omega_0)\) is presented on figure 4 for both specimens.

![Figure 4](image)

**Figure 4.** Dependence of the TI relative error on the experiment parameters \((h, \omega_0)\)

![Figure 5](image)

**Figure 5.** Dependence of the TI for simulated EBSD measurements (a) and for steel EP823 (b) on the experiment parameters \((h, \omega_0)\)**
It can be noticed that the TI behaviour on figure 5 (a) under parameters varying was saved when the new approach for grain structure modelling was utilized. The dependence of TI on experiment parameters, obtained by modelling, was compared with one, calculated for ferritic-martensitic steel EP823 (12Cr-Mo-Si-V-Nb-B) [9]. The EBSD measurements for steel EP823 were performed with the same parameters meanings as in modelling. The dependence of IT on measurement parameters for model experiments, presented in figure 5 (a), was confirmed by the dependence calculated for steel EP823 (figure 5 (b)). The reasonable numerical difference between model and real experiments results of TI estimation can be caused by distinct ODFs and its sharpness of models specimens and steel EP823 (the true ODF of steel is unknown).

4. Conclusions
The improved polycrystalline model with a novel grain structure simulation approach was verified by means of the texture characteristics comparison, restored from the simulated EBSD measurements, for specimens with both grains structure models: novel one with grains in form of ellipses and initial one with grains as circles.

The results of usage of the novel grain structure model allowed to achieved reliable results of texture entities behaviour under parameters varying. Both models considered led to close enough results of ODF, DDDF and TI calculation. The correlation between behaviour of texture entities, restored from simulated EBSD data with both, novel and initial, grain structure models, and really performed EBSD experiments for steel EP823 give us the ability to use novel model for further study of the EBSD parameters choice. Besides the application of the specimen model outlined makes it possible to study the influence of grains elongation factor on the scanning step choice and the reliability of the obtained experiment results. It is also supposed, that the application of the proposed specimen model in the further study of the EBSD experiment parameters choice allows to achieve results of polycrystalline properties calculation, closer to ones, obtained for steel and other real materials.

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