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A novel approach to quantitative analysis of the local deformation in grained structure

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Abstract. Novel technique for identifying and quantification of local deformation phenomena in continuum model of grained solid structure is presented in this paper. We propose a method that combines deformation properties of structure with the changes of grains geometry deformed under the influence of local force. Experimental analyses of grains shapes subjected to a local force show a specific spatially oriented prolongation of grains in direction determined by applied force. However the volume of each grain is retained during the force application in case of plastic deformation. Character of individual grain prolongation depends on the initial shape of grain and direction of loading force. There is a definite relationship between the change in grain shape and nature of the driving deformation force. We contribute to the revealing of mentioned relationship because of we propose and analyze a method for quantification of the effect of grain shape modification on the basis of grain deformation. Quantitative analysis of local deformation in grained structure can be realized in a perspective using mentioned method. Map of local deformation data in grained system can be constructed in this way and next the local deformation dynamics analysis can be performed. However precision of mentioned analysis must be proven by evaluating of its practical predictive performance in future.

1. Introduction

Various technological procedures in the materials preparation are influenced by macroscopic effects of deformation. However these observable macroscopic effects do not reflect local microstructural changes in deformed areas of material in all their diversity. To obtain exact information about local changes in microstructure various more sophisticated methods must be used, for instance methods based on acoustic emission, microhardness measure, dislocations analysis, slip band observation, micromeshes method or macroscopic screw method. But no of these available methods give analytical expressions relating structure parameters and local strain in each position of bulk material volume.

The polycrystalline material is formed from grains having a various shapes. During an applied mechanical loading, according to the different directions and the influences from neighbouring grains, most of grains are submitted to a deformation. The deformation of grain results in a change in orientation and amount of grain surface area which lead to local heterogeneous plasticity. Therefore

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grain surface area and grain edge per unit volume are parameters important in various theories of plasticity as they are generally considered to heterogeneous nucleation sites.

Our work is oriented just on the mathematical treatment of grained structure deformation. Contribution deals with the problem of a grained structure distortion induced by local deformation. We suggest a variable suitable for evaluation of degree of grain surface area orientation with respect to certain vector in three-dimensional space and discuss the relation of this variable to local deformation parameters. Our contribution finishes with a brief commentary on suggested technique of quantitative analysis.

We emphasize that strictly geometric orientation of the grain in three-dimensional space is discussed in our work. We do not discuss orientation of the crystal structure within the grain (even though concept of grain orientation is usually related with crystallographic orientation). A new magnitude κ is defined to evaluate the degree of orientation of the grain surface with respect to a given direction. The presented work aims to find a correlation between the change in the degree of geometrical orientation of a grain and the deformation experienced by it. We study the case of a grain subjected to deformation, and apply the obtained results to the particular case of a randomly oriented grained structure. It is necessary to note that presented paper contains only a mathematical model for the describing the deformation of a fictional, simplified grained structure - no real material is specified, nor is the actual deformation process described. Purely theoretical approach is presented. However it have been shown that such a deformation mechanism, i.e. elongation (or the shortening) of grains under applied load, exists in a real-world material.

2. Quantitative analysis of grains orientation

Grain-surfaces (grain boundaries) play important role in energy balance of grained structure. Loading force causes a specific type of perturbation of this balance in initial grained structure. Therefore it may be supposed that in case of grain deformation certain direction is preferred from the orientation of grain-surface elements point of view. Question is how could be quantified relationship between this preferred orientation of grain-surface area elements and local structure deformation parameters.

Planar character of infinitesimal surface area enables to clearly define orientation of surface element in 3D just by means of the vector $d\vec{S}$. Hence it is possible to easily analyse a sort of "degree" of single surface element orientation in relation to any unit vector $\vec{\tau}$ for example by absolute value of scalar product:

$$\left|\vec{\tau}\cdot d\vec{S}\right| = dS\left|cos\left(\alpha\right)\right| = dS_p \tag{2.1}$$

where α is angle between vectors $\vec{\tau}$ and $d\vec{S}$. This absolute value determines the size of projection of the surface element dS_p to the plane perpendicular to the vector $\vec{\tau}$. Quantity (2.1) calculated per unit surface area of grain, i.e.:

$$\frac{dS\left|cos\left(\alpha\right)\right|}{S}, \tag{2.2}$$

assesses a contribution of the element to a "degree" of whole grain-surface orientation in relation to vector $\vec{\tau}$. We suggest, that for quantitative analysis of grain surface distortion it is required to define a variable κ enabling evaluate "degree" of whole grain-surface orientation in relation to vector $\vec{\tau}$.

Contribution rate of mentioned element to the whole grain-surface orientation can be intuitively proposed by generalization of formula (2.2) as:

$$d\kappa = \frac{dS}{S}\xi\left(\alpha\right),$$

where S is total surface of whole grain and $\xi(\alpha)$ is a function of the angle α. It is advisable to choose the function $\xi(a)$ in such a way that the value κ will be related to an experimentally measurable quantities. We have chosen function $\xi(\alpha)$ in such a way that limit values of variable κ are consistent with values obtained in procedures realized at analysis of particles orientation using Saltykov method [1, 2]. Experimental estimation of grains orientation degree using this method is relatively simple. In consistent with this technique we require:

$$\lim_{\alpha\to\pi/2} \kappa = 1 \ , \qquad \lim_{\alpha\to 0} \kappa = -1 \ . \tag{2.3}$$

So next function can be intuitively used in this case:

$$\zeta(\alpha) = 1 - 2\left|cos(\alpha)\right| \tag{2.4}$$

and contribution $d\kappa$ can be written in the form:

$$d\kappa = \left\{1 - 2\left|cos(\alpha)\right|\right\}\frac{dS}{S} = \frac{dS}{S} - 2\frac{\left|\vec{\tau}\cdot d\vec{S}\right|}{S} \ . \tag{2.5}$$

Degree of whole grain-surface orientation in relation to vector $\vec{\tau}$ can be determined by the integrating of (2.5) over the entire grains surface:

$$\kappa = 1 - 2\frac{1}{S}\int\limits_{(Surface)} \left|\vec{\tau}\cdot d\vec{S}\right| \ . \tag{2.6}$$

We believe that variable κ defined by (2.6) enables to analyze grain-surface area distortion induced by deformation.

3. Relationship between deformation tensor and orientation parameter κ

Consider isotropic, linear elastic material with the grained structure. Generally the parametrization of any grain boundary surface in 3D can be accomplished by spatial coordinates of each points on the surface:

$$X_i = X_i(u,v), \text{ where } i = 1, 2, 3. \tag{3.1}$$

and u, v are parameters that changes in defined intervals. Therefore the position vectors of each points on the surface of single grain boundary with any possible shape in undeformed configurations can be written as:

$$\vec{R}(u,v) = \left[X_1(u,v), X_2(u,v), X_3(u,v)\right] \quad , \quad u \in \langle u_1, u_2\rangle \quad , \quad v \in \langle v_1, v_2\rangle \ . \tag{3.2}$$

Let the position vectors of each points on the surface of the same grain in deformed configurations are:

$$\vec{r}(u,v) = \left[x_1(u,v), x_2(u,v), x_3(u,v)\right] \quad , \quad u \in \langle u_1', u_2'\rangle \quad , \quad v \in \langle v_1', v_2'\rangle \ . \tag{3.3}$$

In general case, any 3D deformation can be described by a 3x3 deformation tensor $\vec{\vec{\varepsilon}}$. Using notation mentioned above the grain linear deformation (for small strain) can be expressed as anisomorphic linear transformation:

$$\vec{r} = \vec{\vec{\varepsilon}}\cdot\vec{R}, \quad \text{or} \quad x_i = \varepsilon_{ij} X_j, \tag{3.4}$$

where i, j = 1, 2, 3 and ε_{ij} are coefficients of deformation tensor. It is no problem to verify that $\varepsilon_{ij} = \delta_{ij}$ in undeformed case (where δ_{ij} is Kronecker symbol). We used typical Einstein`s summation convention in the second formula in (3.4) whereby when an index variable appears twice in a single term it implies summation of that term over all the values of the index.
Considering transformation (3.4) when calculating the orientation parameter (2.6) we get:

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$$\kappa_{defor} = 1 - 2\frac{\int\limits_{(Surface)} \left| \left(\vec{\vec{\sigma}}^T \cdot \vec{\tau} \right) \cdot d\vec{S}_{undefor} \right|}{\int\limits_{(Surface)} \left| \vec{\vec{\sigma}} \cdot \vec{\rho} \right| dS_{undefor}} \tag{3.5}$$

where $\vec{\vec{\sigma}}$ is a tensor coefficients of which are related to coefficients of deformation tensor $\vec{\vec{\varepsilon}}$:

$$\sigma_{wm} = (-1)^{w+m} \, det\left(\vec{\vec{\varepsilon}}_{mw} \right). \tag{3.6}$$

$det\left(\vec{\vec{\varepsilon}}_{mw}\right)$ is the minor (or subdeterminant) of matrix of the deformation tensor $\vec{\vec{\varepsilon}}$. So it is easily to show that coefficients of tensor of grain surface deformation can be found as:

$$\sigma_{wm} = \varepsilon_{ik}\varepsilon_{jn} - \varepsilon_{in}\varepsilon_{jk}, \tag{3.7}$$

We note that $\vec{\vec{\sigma}}^T$ in formula (3.5) is tensor that is transposed to the tensor $\vec{\vec{\sigma}}$ determined by (3.6). It can be seen from (3.5) that in general the transformation of parameter κ during grain deformation appears to be relatively complicated and we will not examine its mathematical properties in detail. However, it should be noted that we integrate over the surface of undeformed grain in the formula (3.5). So to determine the value κ in deformed configuration we need to know only the shape of undeformed grain and coefficients of deformation tensor ε_{ij}. Therefore we believe, that κ could be an acceptable scalar variable suitable for the quantitative evaluation of grain-surface distortion during local deformation of grained structure.

4. Monte Carlo simulation of the parameter κ - the case of "random" grained structure

Integrals in formula (3.5) must be integrated over the entire surface of grains boundaries if the whole grained structure orientation κ is evaluated. For the calculation purposes this integral can be transformed to summation over the small areas placed around whole grains boundaries surface (infinitely small in the ideal case). So we get:

$$\kappa_{defor} \approx 1 - 2\frac{\sum_{i=1}^{N} \left| \left(\vec{\vec{\sigma}}^T \cdot \vec{\tau} \right) \cdot \vec{S}^{(i)} \right|}{\sum_{i=1}^{N} \left| \vec{\vec{\sigma}} \cdot \vec{\rho}^{(i)} \right| S^{(i)}}. \tag{4.1}$$

where $\vec{\tau} = \left[\tau_1, \tau_2, \tau_3\right]$ is any unit vector (i.e. $\tau_1^2 + \tau_2^2 + \tau_3^2 = 1$) and $\vec{\rho}^{(i)}$ is unit vector perpendicular to the *i*-th grain-surface element of undeformed grain:

$$\vec{S}^{(i)} = \vec{\rho}^{(i)} S^{(i)}. \tag{4.2}$$

Vector $\vec{\rho}^{(i)}$ can be written in the form:

$$\vec{\rho}^{(i)} = \left[sin\left(\eta^{(i)}\right) cos\left(\chi^{(i)}\right), sin\left(\eta^{(i)}\right) sin\left(\chi^{(i)}\right), cos\left(\eta^{(i)}\right) \right] \quad , \quad \chi^{(i)} \in \langle 0, 2\pi \rangle, \quad \eta^{(i)} \in \langle 0, \pi \rangle$$

while angles $\eta^{(i)}$ and $\chi^{(i)}$ determines orientation of the *i*-th grain-surface element and then:

$$\vec{S}^{(i)} = \left[S_1^{(i)}, S_2^{(i)}, S_3^{(i)} \right] = \left[S^{(i)} sin\left(\eta^{(i)}\right) cos\left(\chi^{(i)}\right), S^{(i)} sin\left(\eta^{(i)}\right) sin\left(\chi^{(i)}\right), S^{(i)} cos\left(\eta^{(i)}\right) \right]. \tag{4.3}$$

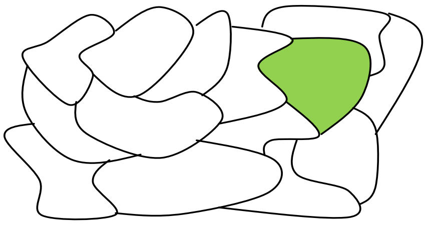


Figure 1. Scheme illustrating a view on a grained structure cross-section (for example on metallographic cut). Cross-section of some individual grain is colored.

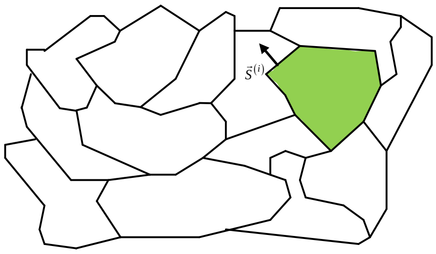


Figure 2. Scheme illustrating a view on the model of the same grained structure cross-section. Scheme demonstrates the replacement of grain surface by small flat areas.

If we use result (3.7) and notations (4.3) sums in the formula (4.1) can be easy calculated. As can be shown the problem of grained structure orientation can be formulated mathematically as random matrix problems. In this sense, the formula (4.1) can be rewritten to the form:

$$\kappa_{defor} \approx 1-2\frac{\sum_{i=1}^{N}\left(S^{(i)}\left|\sum_{n=1}^{3}\tau_n \, det\, \tilde{A}_n^{(i)}\right|\right)}{\sum_{i=1}^{N}\left(S^{(i)}\sqrt{\sum_{n=1}^{3}\left(det\, \tilde{A}_n^{(i)}\right)^2}\right)} \qquad \ldots \quad n=1,2,3 \tag{4.4}$$

where $det\, \tilde{A}_n^{(i)}$ is determinant of random matrix $\tilde{A}_n^{(i)}$ with coefficients:

$$\tilde{A}_{nmk}^{(i)} = \varepsilon_{mk}\left(1-\delta_{m,n}\right)+\frac{1}{2}\delta_{m,n}\left\{\left[1+(-1)^{\alpha_k}\right]sin\left(\eta^{(i)}\right)cos\left(\chi^{(i)}\right)+\left[1+(-1)^{k}\right]sin\left(\eta^{(i)}\right)sin\left(\chi^{(i)}\right)+ \right.$$
$$\left. +\left[1+(-1)^{\beta_k}\right]cos\left(\eta^{(i)}\right)\right\} \tag{4.5}$$

and:

$$\alpha_k = \sum_{\nu=1}^{k}\frac{1+(-1)^{\nu}}{2} \quad , \beta_k = \sum_{\nu=1}^{k}\frac{1-(-1)^{\nu}}{2} \quad , \quad \ldots \quad n,m,k=\{1,2,3\}.$$

Formula (4.4) can be imposed and smartly used in the formal mathematical notation as well as numerical implementation of considered approximation approach.

We suppose calculate degree of whole grained structure orientation κ in relation to any unit vector $\vec{\tau}$ by means of the formula (4.4) while sums in the numerator and denominator in the second member on the right side of this formula can be determined step by step. Any randomly oriented surface element of grain boundary $S^{(i)}$ in the given bulk sample with grained structure can be included into the calculation of κ if corresponding parameters $\eta^{(i)}$ and $\chi^{(i)}$ will be applied. Therefore random values of angles $\eta^{(i)}$ and $\chi^{(i)}$ should be substituted step by step into formula (4.5) when the calculation progress.

5. Investigation of the simulation procedure

In this section we present investigation of computational stability of procedure described above. Consider random grained structure with uniform distribution of parameters $\eta^{(i)}$ and $\chi^{(i)}$. Values of these parameters were generated by random number generator character of which was tested (see Figure 3). As can be seen from the Figure 3 no direction is preferred from the flat element $S^{(i)}$ orientation point of view. Let the scalar variable $\kappa = 0$ for this grained structure in undeformed state. Consider for example the deformation of mentioned structure described by next deformation tensor:

$$\vec{\vec{\varepsilon}}_{defor} = \begin{pmatrix} 0.8\,, & 1.2\,, & 1.45 \\ 0.42\,, & 0.5\,, & 0.62 \\ 1.09\,, & 2.22\,, & 0.722 \end{pmatrix}. \tag{5.1}$$

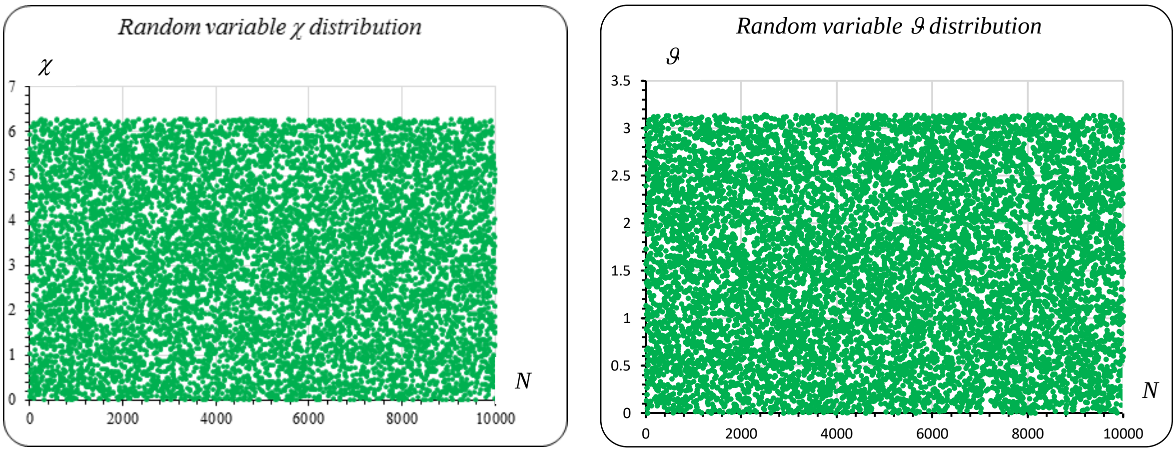
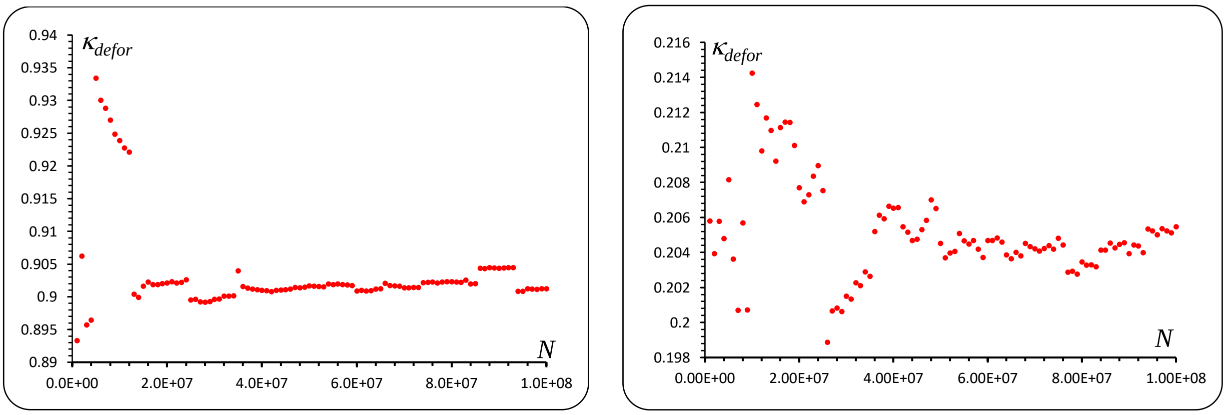


Figure 3. Random number generator test. Each point on graphs corresponds to generated value of the parameter.

Degrees of whole grained structure orientation κ_{defor} in relation to a few arbitrary chosen vectors $\vec{\tau}$ were calculated by Monte Carlo simulation using the formula (4.4).
Results of the simulation are shown in the Figure 4. As can be seen from presented graphs if the number of considered flat elements N is increasing the variance of calculating values κ_{defor} decreases. Computational test was carried out up to $N = 10^8$.



a) $\vec{\tau} = [0,0,1]$, limit value $\kappa_{defor} = 0.9013$

b) $\vec{\tau} = [1,0,0]$, limit value $\kappa_{defor} = 0.2055$

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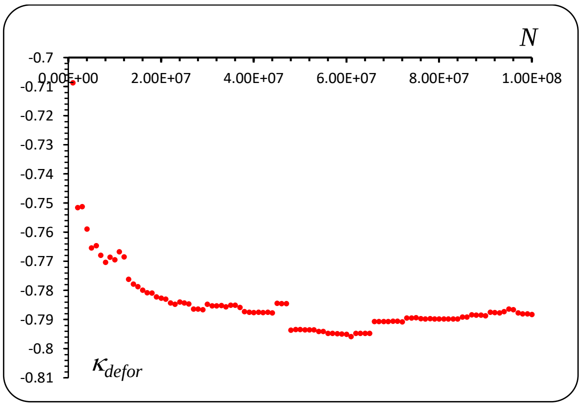
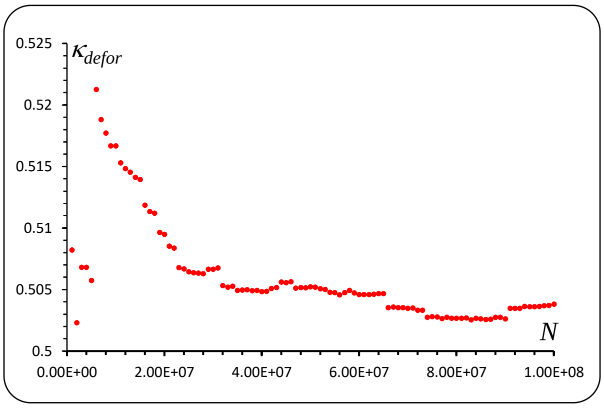
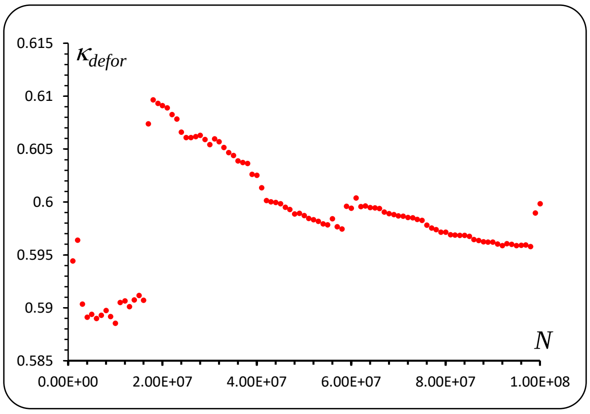


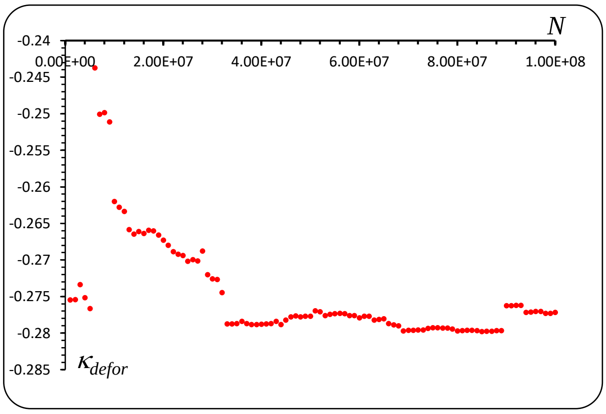
c) $\vec{\tau} = [0,1,0]$, limit value $\kappa_{\text{defor}} = -0.78816$



d) $\vec{\tau} = [0.5,0.5,0.70711]$, limit value $\kappa_{\text{defor}} = -0.5038$



e) $\vec{\tau} = [0.171,0.296,0.94]$, limit value $\kappa_{\text{defor}} = 0.599$



f) $\vec{\tau} = [0,0.707,0.707]$, limit value $\kappa_{\text{defor}} = -0.277$

Figure 4. Result obtained by Monte Carlo simulation of parameter κ for the deformed grained structure described by deformation tensor (5.1). Graphs show calculated value of parameters κ_{defor} as a function of considered number of randomly oriented grains boundaries elements N in the stochastic model of grained structure illustrated in the Figure 2. Presented results clearly demonstrate the convergence of calculated values κ_{defor} when the simulation is running. This fact suggests the applicability of proposed procedure for investigation of local deformation in real grained structures.

6. Conclusion

In this paper values of parameteters established in stereology are used to extend the results of stereological measurements to provide a predicts the local deformation of grained structure. Orientation of grains in a microstructure reflects this deformation in terms of quantities that can be directly measured in microstructures by means of stereological methods. This is illustrated with a set of simulations that successfully tests our predictions.

Generally one can easily understand that there is a correlation between the change in the grain orientation and grain deformation [3, 4]. This correlation was mathematically demonstrated in our work. Indeed, the expression (3.5) allows one to investigate this correlation. Finally, if we interpret the quantity κ as the degree of grain orientation corresponding with the value measured at Saltykov method, the analysis of local deformation could be easily realized experimentally on the basis of our results. As an illustration we have shown the applicability of our results for random model of grained structure. This specific case of model have used here because of its simplicity but we believe that our method can be applied also for other models.

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