E14-2002-49

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MODEL INVESTIGATION OF THE GRAIN NUMBER TO APPLY QUANTITATIVE TEXTURE ANALYSIS AVERAGING

Submitted to «physica status solidi»

1. INTRODUCTION

One of the widely used methods to calculate physical properties is the averaging of single crystal properties with an orientation distribution function (ODF) [1, 2]. However, the limitations to apply averaging procedures to real materials are still unclear. A number of grains do not influence the mathematical definition of the ODF, nevertheless, intuitively clear that, the averaging procedure implies a "large" number of grains to make sense. In this paper the influence of the grain statistics and the grain area distribution on averaging accuracy were considered. For this purpose a grain microstructure has been simulated. Comparable simulations carried out earlier did not take into account three-dimensional random rotations distributed according to a known law [3-4]. In this paper it is proposed to simulate the grain microstructure according to Voronoi approach and three-dimensional random rotations distributed with known law simultaneously. From our point of view this model is rather close to a real polycrystalline aggregate. Using Voronoi method we followed the procedures described in [5-7].

First, the main definitions of quantitative texture analysis are given and the usual averaging procedure is described. In the next section we present outlines of the applied algorithm to generate spatial microstructure. Afterwards, the simulation of random rotations with known distribution according to Roberts approach [8] is described. Finally, numeric examples illustrating the influence of grain statistics and grain area distributions on the elastic constants of cubic and hexagonal textured materials are presented.

2. FUNDAMENTALS

Denote by dV volume of all crystallites in a sample which possess an orientation g within orientation region dg, and by V the total sample volume, then the orientation distribution function $f(g)$ is defined by [1]:

$$f(g)dg = \frac{dV(g)}{V}. \tag{1}$$

All rotations form the rotation group SO(3). The ODF is defined on the rotation group SO(3). The ODF defined by (1) implies infinite number of orientations and we will call it "continuous" ODF $f^c(g)$ with normalization property:

$$\frac{1}{8\pi^2}\int_{SO(3)} f^c(g)dg\,. \tag{2}$$

However, a real sample consists of a finite number of grains. If the number of grains in specimen is N, then the specimen is described by the "discrete" ODF $f^d(g,N)$ in terms of δ - functions on SO(3):

$$f^d(g,N) = \frac{1}{V}\sum_{n=1}^{N} V_n \delta\left(g g_n^{-1}\right), \quad V = \sum_{n=1}^{N} V_n\,, \quad \frac{1}{8\pi^2}\int_{SO(3)} \delta\left(g g_n^{-1}\right)dg = 1. \tag{3}$$

Let $\bar{y}$ be the unit vector in the sample coordinate system, $\vec{h}$ be the unit vector in single crystal coordinate system, $dV(\vec{h} \parallel \bar{y})$ is the volume fraction of the sample for which the crystallographic direction $\vec{h}$ coincides with $\bar{y}$ in $[\bar{y}, \bar{y} + d\bar{y}]$. Then the pole figure $P_h(\bar{y})$ is a function conformed to condition [1]:

$$\frac{1}{4\pi} P_h(\bar{y})d\bar{y} = \frac{dV(\vec{h} \parallel \bar{y})}{V}. \tag{4}$$

The PFs are defined on the sphere S^2 with the normalization property [1, 2]:

$$\frac{1}{4\pi}\int_{S^2} P_h(\bar{y})d\bar{y} = 1. \tag{5}$$

The connection between the ODF and the PFs is given by the integral [2]:

$$P_h(\bar{y}) = \frac{1}{2\pi}\int_0^{2\pi} f\left(\{\vec{h},\varphi\}^{-1}\{\bar{y},0\}\right)d\varphi\,. \tag{6}$$

If material has crystal symmetry with point group $R_B = \{r_{B_i}, i = 1,..., M_B\}$ and sample symmetry with point group $R_A = \{r_{A_i}, i = 1,..., M_A\}$, where $G_B = \{g_{B_i}, i = 1,..., N_B\}$, $G_A = \{g_{A_i}, i = 1,..., N_A\}$ are theirs sub-groups belonged to rotation group SO(3) then PF and ODF are conformed to the following symmetry conditions:

$$f(g) = f(g_{B_j} \cdot g \cdot g_{A_i}),\ j = 1,...,N_B,\ i = 1,...,N_A;$$

$$P_h(\bar{y}) = P_{r_{B_j} h}(r_{A_i} \bar{y}),\quad j = 1,...,M_B,\ i = 1,...,M_A. \tag{7}$$

To satisfy these conditions, the equation (6) should be rewritten in the form [2]:

$$P_h^s(\bar{y}) = \frac{1}{M_A M_B} \frac{1}{2\pi} \sum_{i=1}^{M_A} \sum_{j=1}^{M_B} \int_0^{2\pi} f\left(\left\{r_{B_j} \vec{h}, \varphi\right\}^{-1} \left\{r_{A_i} \bar{y}, 0\right\}\right) d\varphi = \frac{1}{M_A M_B} \sum_{i=1}^{M_A} \sum_{j=1}^{M_B} P_{r_{B_j} \cdot h}(r_{A_i} \bar{y}). \tag{8}$$

The approach for calculation of mean physical properties, that does not make any speculations on the sample internal microstructure, is the arithmetic averaging of the single crystal properties E with the ODF $f(g)$ as a weighting function [1, 2]:

$$\bar{E}^a = \frac{1}{V} \int_V E(\bar{r}) dV = \frac{1}{V} \oint_g E(g) \int_{V(g)} dV = \int_g E(g) f(g) dg. \tag{9}$$

The averaging procedure (9) implies an infinite number of grains. This formula takes into account the ODF definition (1) and moreover the relations $E(\bar{r}) = E(g^{-1} \cdot h) = E(g)$. However, any real sample or product possesses a finite volume and consequently a limited number of grains. Moreover, grains may be unevenly distributed in the considered volume. Both these aspects should be taken into account for the accurate application of (9). Such investigations are the purpose of this paper.

3. SIMULATION OF GRAIN MICROSTRUCTURE

In order to generate microstructure pattern the cells (Voronoi) model [5, 6] was used. First, random points P_1, P_2,..., P_N are picked in space. Subsequently, space is divided into cells (grains) C_1, C_2, ..., C_N according to the rule: C_i contains all points in space closer to P_i than to any P_j $(j \neq i)$. In the Voronoi model C_i is a convex polyhedron called by Voronoi polyhedron if dimension of space D ≥ 3 and C_i is a convex polygon (Voronoi polygon) if D = 2. P_i is called the center of C_i. Connecting all P_i whose Voronoi cells have common boundaries, a system of tetrahedrons/triangles called by Delaunay tessellation (triangulation in case D = 2) can be obtained. For application of the Voronoi model to generate of grain microstructures, P_i represents the model

location of the original nucleus or seed crystal from which the cell (grain) grew. One assumes for such application the following:

(i) the seeds for all crystals start growing at the same instant;

(ii) seeds grow at the same rate in all directions (i.e., as spheres); and

(iii) seeds stay fixed in space without pushing apart as they grow into contact.

Very effective algorithms to simulate planar Voronoi diagram are based on three-dimensional convex hull [9-10]. The connection between convex hull in space D+1 and Delaunay tessellation in space D is shown in [9]. We used the "divide-and-conquer" algorithm [11] improved by K. Sugihara [10] to construct such convex hull. This algorithm runs optimal O(n log n) time [11] and employs exact arithmetic to avoid inconsistency caused by numerical errors. The coordinates of the input points P_i are integers. The topology of the microstructure for a number of grains N approximated as a Voronoi tessellation is presented in Fig. 1.

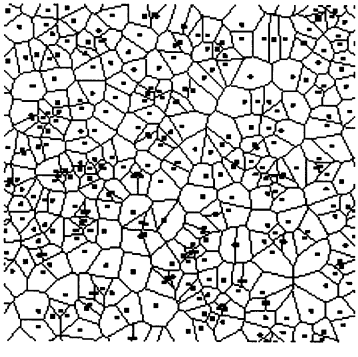


Fig. 1. The example of plane Voronoi tesselation.

In Fig. 2, the examples of microstructure or planar Voronoi diagram constructed for N = 5000 random uniformly distributed input points and for N = 5000 input points randomly distributed according to normal and exponential laws are given.

On the basis of planar grain microstructure grain area distributions can be calculated. These distributions for microstructures constructed for N = 5000 input points randomly distributed according to different laws are presented in Fig. 3. It has been calculated by averaging of 20 statistical realizations of the algorithm for Voronoi diagram construction. The grain area distribution presented in Fig. 3 for input points distributed according to the exponential law is in good qualitative agreement with the distribution obtained for microstructure measured by Electron Back Scattered

Diffraction [12]. This confirms the reliability of the Voronoi approach to simulate grain microstructures.

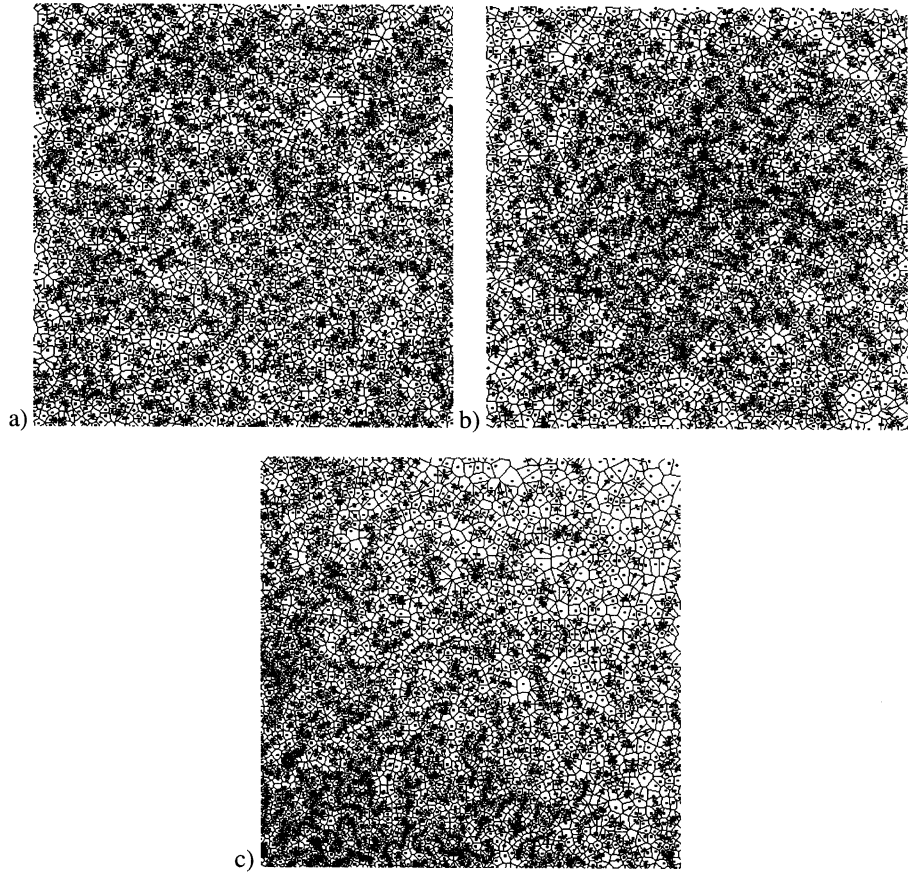


Fig. 2. Voronoi 2D diagrams - microstructures constructed for N = 5000 input points random distributed a) uniformly; according to b) normal law, c) exponential law.

It has been shown in [13, 14] that Voronoi cell area distribution can be described by generalized gamma-distribution:

$$f(x) = rb^{q/r} x^{q-1} \exp(-bx^r) / \Gamma(q/r),\ r>0,\ b>0,\ q>0. \tag{10}$$

From the other hand, the authors of paper [15] state that gamma distribution:

$$(r=1)\ \ f(x) = b^q x^{q-1} \exp(-bx) / \Gamma(q) \tag{11}$$

as well as lognormal and Maxwell distributions can also be used.

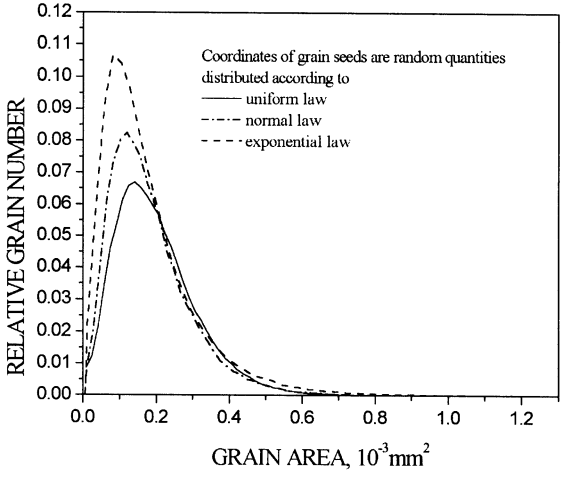


Fig. 3. Grain-area distributions (histograms) for microstructures represented in Fig. 2.

It should be noted that there are other algorithms (for example Anderson [3, 4] or Johnson-Mehl model [5, 6]) to generate spatial microstructures, but it turns out, that qualitatively average characteristics like grain area distributions produced within these models are similar to those produced by the Voronoi model.

4. SIMULATION OF THREE - DIMENSIONAL ROTATIONS

To investigate the influence of a grain number on the elastic constants an ensemble of individual orientations $g_n \in SO(3)$ for N grains was simulated according to the approach of Roberts *et. al.* [8]. This approach was already used in [16] to investigate optimal grid parameters for texture measurements. Following [8], the ensemble g_n is distributed according to the Brownian motion law on SO(3). The orientation:

$$g = [\omega, \vec{n}] = [\omega, \vartheta, \varphi], \quad g \in SO(3), \quad 0 \le \omega < 2\pi, \quad 0 \le \vartheta \le \pi, \quad 0 \le \varphi \le 2\pi,$$

can be presented as a point on the unit hypersphere S^3 in the four-dimensional Euclidean space R^4 with hyperspherical coordinates:

$(r,\psi,\vartheta,\varphi) \equiv (\psi,\vartheta,\varphi)$, $r=1$, $0 \le \psi \le \pi$,

where $2\psi = \omega$. The Euclidean coordinates of this point are $\vec{r} = (x_1, x_2, x_3, x_4)$, $\vec{r} \in S^3 \subset R^4$, $\sum_{i=1}^{4} x_i^2 = 1$. If one considers a sequence of t rotations through a fixed angle Λ about a randomly oriented axis with random direction, and Brownian motion starts at $g = \{0°,0°,0°\}$ ($g \in SO(3)$), then the distribution density $\rho_t(\vec{r})$, $\vec{r} \in S^3 \subset R^4$ after t rotations at special conditions $t \to \infty$, $\Lambda \to 0$, $\Lambda^2 t \to const$ can be written as follows [8, 16]:

$$\rho(\vec{r}) = \frac{1}{2\pi^2} \sum_{l=0}^{\infty} (2l+1) \exp\{-l(l+1)D\} \frac{\sin\left((2l+1)\omega/2\right)}{\sin\left(\omega/2\right)}, \qquad D = \frac{\Lambda^2 t}{6}. \tag{13}$$

The distribution corresponding to (13) on the sphere $S^2 \subset R^3$ is [16]:

$$\rho(\vec{y}) = \frac{1}{4\pi} \sum_{l=0}^{\infty} (2l+1) \exp\{-l(l+1)D\} P_l(\cos\beta), \quad \vec{y} = (\beta,\varphi) \in S^2, \tag{14}$$

where $P_l(\cos\beta)$ are Legendre polynomials, D is parameter connected to the strength of the texture. To generate the ensemble of g_n distributed with density (13) choose $\Lambda_0 << 1$ and $t_0 >> 1$ so that $D = \Lambda_0^2 t_0 / 6$ is valid. Besides, an appropriate symmetrization (7) is required to obtain the actual ODF and PFs. After subjecting the initial orientation $g = \{0°,0°,0°\}$ to a series of rotations through a fixed angle Λ around the random axis we obtain the ensemble of g_n distributed with density (13), which is the texture component with sharpness D. The simulated ensemble g_n can be considered as "sample" with N grains described by a "discrete" ODF $f^d(g,N)$. Using formula (6), the corresponding PFs $P_h^d(\vec{y},N)$ can be calculated. Including also information about the experimental conditions an experimental PFs $P_h^e(\vec{y},N)$ can be calculated as well [16]. To evaluate the quality of the experimental PFs the R-factor is introduced by [16]:

$$R \approx \frac{1}{M} \sum_{m=1}^{M} RP\left(\varepsilon, P_h^c(\vec{y}_j), P_h^{e,m}(\vec{y}_j,N)\right), \tag{15}$$

where $P_h^{e,m}(\bar{y},N)$ is the m-th independent realization of the simulated experimental PF, $M=10$ is the number of independent realizations, $P_h^c(\bar{y})$ is the known distribution of "continuous" PF. The *RP* factor can be determined as following [17]:

$$RP=\sum_{j=1}^{J}100\%\Theta[\varepsilon,P_h(\bar{y}_j)]r_j \Big/ \sum_{j=1}^{J}\Theta[\varepsilon,P_h(\bar{y}_j)], \tag{16}$$

where $r_j=\left|P_h^c(\bar{y}_j)-P_h^{e,m}(\bar{y}_j)\right|/P_h(\bar{y}_j)$, $\Theta(\varepsilon,x)=\begin{matrix}0,x\le\varepsilon\\1,x>\varepsilon\end{matrix}$.

In Fig. 4 the PFs simulated for cubic material with different grain number and a single component texture model are given. The center of the component is $g=\{0°,0°,0°\}$ and width parameter $D\approx 0.042$ was determined using $\Lambda_0=0.025$ and $t_0=400$. This corresponds to *HWHM* $\approx 19.7°$ of the texture component. As can be seen from Fig. 4, increasing the number of grains minimizes the R- factor and makes simulated PFs closer to "continuous" PFs. Fig. 5 shows the dependence between pole figures and texture sharpness, controlled by the width parameter D.

5. INFLUENCE OF GRAIN NUMBER AND GRAIN AREA DISTRIBUTION ON THE ELASTIC CONSTANTS OF TEXTURED MATERIALS

To underline the importance of grain area distributions for the modeling, the results for models with equal volume grains are presented first.

The properties with "discrete" ODF (3) can be found in the framework of an equal grain model ($V_n=V_0=V/N$, $n=1,\ldots,N$) as follows:

$$E_{ijkl}=\sum_{n=1}^{N}E_{ijkl}(g)f^d(g,N)=\frac{1}{N}\sum_{n=1}^{N}E_{ijkl}(g_n), \tag{17}$$

where $E_{ijkl}(g_n)$ is the property of grain n. Considering the more realistic case where the grain volumes are distributed according to some law, the properties with "discrete" ODF (3) can be found as follows:

$$E_{ijkl} = \sum_{n=1}^{N} E_{ijkl}(g) f^{d}(g,N) = \frac{1}{V} \sum_{n=1}^{N} E_{ijkl}(g_n) V_n , \qquad (18)$$

where V is the sample volume, V_n is the volume of grain n, $E_{ijkl}(g_n)$ is the property of grain n.

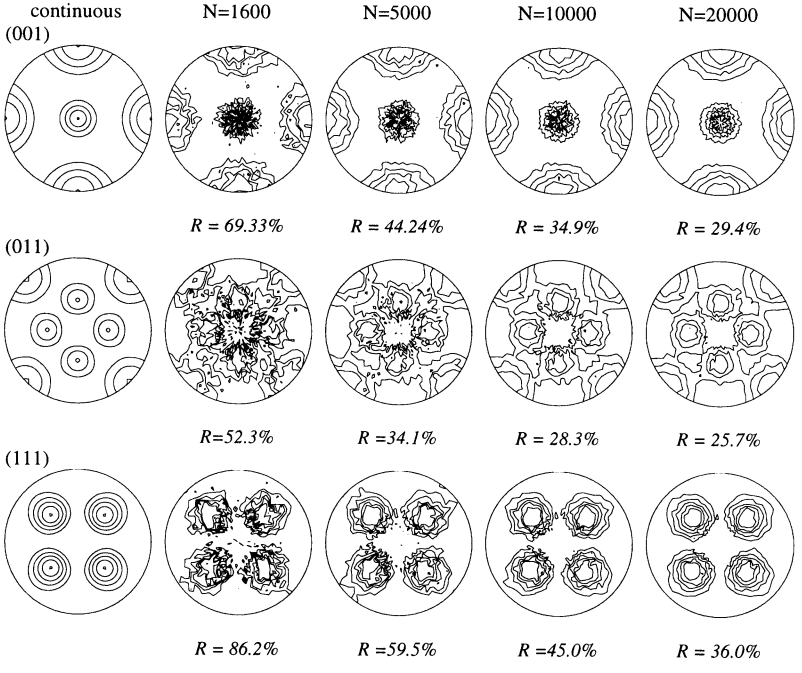


Fig. 4. Pole figures of cubic material simulated on grid with step 5° for the texture model g = {0°,0°,0°} $D \approx 0.042$ ($HWHM \approx 19.7°$): first column is " continuous " PFs, last columns are "discrete" PFs simulated for samples with different number of grains. Contours are for PF(001) 1, 2, 3, 4 mrd; for PF(011) 1, 1.5, 2 mrd; for PF(111) 1, 1.5, 2, 2.5, 3 mrd.

Ensembles of individual orientations having gaussian distributions with center $g = \{0^{\circ},0^{\circ},0^{\circ}\}$, width parameter D=0.042 ($HWHM$=19.7°, $\Lambda_0 = 0.025$, t_0=400) and $g = \{0^{\circ},0^{\circ},0^{\circ}\}$, D=0.0192 ($HWHM$=13.6°, $\Lambda_0 = 0.012$, t_0=800) were simulated. Subsequently, the Young's module was determined assuming equal grain size as follows:

$$E_{1111}(N) = \frac{1}{M}\sum_{m=1}^{M} E_{1111}^{m}(N), \tag{19}$$

where $E_{1111}^{m}(N) = \frac{1}{S_{1111}^{m}}$, $S_{1111}^{m} = \frac{1}{N}\sum_{n=1}^{N} S_{ijkl}(g_n^m)$, $S_{ijkl}(g)$ is the component of compliance tensor given in single crystal coordinate system, $E_{1111}^{m}(N)$ is the result of the m-th statistical realization of the algorithm to simulate a set of individual orientations g_n^m, M is the number of independent realizations of this algorithm.

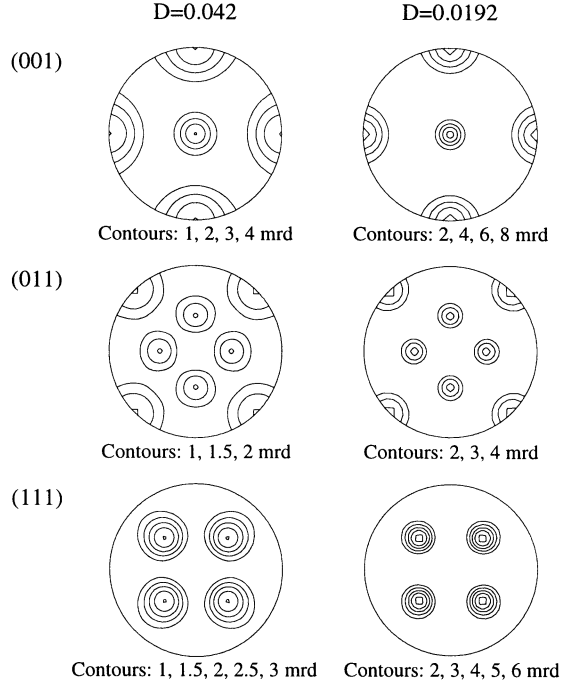


Fig. 5. The "continuous" pole figures of cubic material with different width parameter D. The "discrete" pole figures reveal the same dependence on texture sharpness.

In case of grain volume distributions Young's module was determined as a averaging of M independent statistical realizations of the algorithm to simulate a set of individual orientations, and the algorithm for Voronoi diagram constructing. That is why the

results of Young's module calculations do not depend on statistical realization of these algorithms. The result of m-th realization in this case was determined as follows:

$$E^m_{1111}(N) = \frac{1}{S^m_{1111}},\ S^m_{1111} = \frac{1}{F}\sum_{n=1}^{N} S_{ijkl}(g^m_n)F_n, \tag{20}$$

where F is sample area, F_n is the area of grain n.

Relative error of Young's module calculation was determined as a function of a number of grains in "sample":

$$\delta = \frac{|E_{1111}(N) - E^R_{1111}|}{\min(E_{1111}(N), E^R_{1111})}, \tag{21}$$

where E^R_{1111} is Young's module calculated by Reuss approximation (i.e. with assumption $N \to \infty$):

$$E^R_{1111} = \frac{1}{< S_{1111} >},\ < S_{1111} >= \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} S_{1111}(\alpha,\beta,\gamma) f^c(\alpha,\beta,\gamma)\sin\beta d\alpha d\beta d\gamma, \tag{22}$$

where $S_{1111}(\alpha,\beta,\gamma)$ is the component of compliance tensor given in single crystal coordinate system, $f^c(\alpha,\beta,\gamma)$ is a "continuous" ODF.

The results of Young's module calculation for copper and zinc with different texture model are presented in Tables 1-2. The calculations were carried out without taking into account grain area distributions. As can be seen in the Tables 1-2, relative error δ decreases with increasing the number of grains in the "sample". Moreover, the sharper texture of material the weaker is the dependence of elastic properties from the number of grains.

Subsequently, we considered the grain area distribution. The grain microstructure was simulated as described in the section 3. Cases with random uniform distribution of input points as well as cases with normal and exponential law distributions were studied. The calculations of Young's module were carried out for the two texture models already mentioned above. Young's module was determined according to (20) and also evaluated according to (21). The relative error δ of Young's module calculation as a function of the grain number has been determined with and without taking the grain area distribution into account. The dependencies $\delta(N)$ for copper and

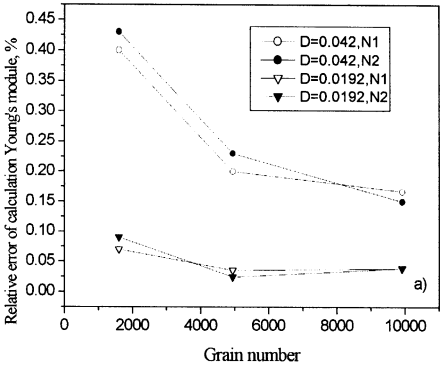
Table 1. Young's module of the textured polycrystalline, (g = {0°,0°,0°}, *D*=0.042), M=10

Grain number, N	Young's module E(N), GPa	δ, %
Copper, Young's module (Reuss) = 85.81GPa		
1600	85.47	0.4
5000	85.61	0.2
10000	85.67	0.16
Zinc, Young's module (Reuss) = 121.61GPa		
1600	121.53	0.07
5000	121.57	0.03
10000	121.59	0.02

Table 2. Young's module of the textured polycrystalline (g = {0°,0°,0°}, *D*=0.0192), M=10

Grain number, N	Young's module E(N), GPa	δ, %
Copper, Young's module (Reuss) = 76.27GPa		
1600	76.22	0.07
5000	76.243	0.035
10000	76.241	0.038
Zinc, Young's module (Reuss)= 122.68GPa		
1600	122.67	0.012
5000	122.68	2×10^{-4}
10000	122.68	2×10^{-4}

zinc are compared with those calculated without taking the grain area distribution into account (see Fig. 6). As can be seen from Fig. 6 the influence of the grain area distribution increases the relative error of Young's module calculation. With increasing a number of grains N in sample the difference between the calculations with and without taking into account these distribution decreases and can be neglected for N = 8000 (copper) and N = 10000 (zinc) in case of texture model with D = 0.042. For sharper texture this difference decreases as well and can be neglected for smaller number of grains (N = 4000, N = 5000, respectively).



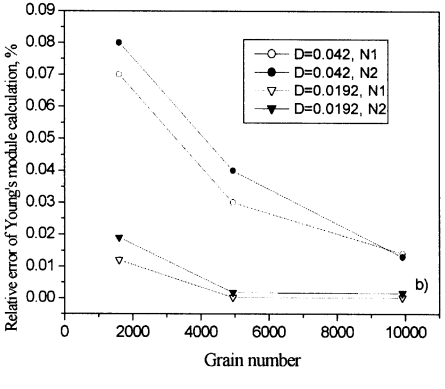


Fig. 6. The relative error of Young's module calculation evaluated for two texture model g = {0°,0°,0°} (D=0.042, D=0.0192) as a function of grain number without (calculation N1) and with (calculation N2) taking the grain area distribution into account for a) copper, b) zinc.

The results of Young's module calculations weakly depend on distribution of input points (grain seeds).

6. CONCLUSIONS

The used solid state model, which is a combination of three-dimensional random rotations with known distribution and Voronoi tessellation, is very close to a real polycrystalline. The obtained results of Young's module calculation do not depend on

the statistical realization of Voronoi and Roberts algorithms, but depend on the number of grains and texture appearance. It is established that the grain area distribution does not depend on the distribution of grain seeds (input points). The algorithm to evaluate limitations for arithmetic averaging technique is pointed out. These limits were determined for selected examples. The minimum number of grains for conventional averaging is about 8000 in the case of copper and about 10000 in the case of zinc. Taking into account the influence of grain area distributions increases the error of elastic property calculation.

Acknowledgments

The authors are grateful to Prof. K. Sugihara for making his perfect software available and applicable for our investigations and to Dr. V. Luzin for valuable discussions and permanent interest in this work. We would like to express our special thanks to Dr. Ullemeyer for very useful remarks.

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Received on March 18, 2002.

Лычагина Т. А., Николаев Д. И.
Е14-2002-49

Модельное исследование применимости усреднений
в количественном текстурном анализе

Одним из наиболее важных применений функции распределения ориентаций (ФРО) является вычисление физических свойств поликристаллов путем усреднения свойств составляющих их кристаллитов. В данной работе исследуется вопрос о количестве зерен в образце, необходимом для проведения усреднений с ФРО с требуемой точностью. Для этого смоделирована микроструктура поликристалла на уровне зерен и каждому зерну присвоена случайная ориентация. Для моделирования микроструктуры использовано разбиение Вороного, а для генерирования случайных ориентаций, распределенных по известному закону, применялся подход Робертса. Для наборов зерен с известными объемами и ориентациями, с одной стороны, и известными ФРО, с другой, были вычислены упругие модули. Оказалось, что оба подхода приводят к одинаковым значениям упругих модулей при количестве зерен в образце, стремящемся к бесконечности. Разница между результатами расчета с учетом и без учета распределения зерен по площадям значительна при числе зерен, меньшем 8000 для материала с кубической симметрией и 10000 для материала с гексагональной симметрией.

Работа выполнена в Лаборатории нейтронной физики им. И. М. Франка ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна, 2002

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E14-2002-49

Model Investigation of the Grain Number
to Apply Quantitative Texture Analysis Averaging

One of the most important applications of an orientation distribution function (ODF) is the computation of physical property averages. A number of grains in a sample is investigated in order to the averaging with a use of ODF reasonable from the accuracy point of view. For that, a microstructure pattern has been generated and a random orientation with known distribution has been assigned to each grain. In order to generate microstructure patterns, Voronoi cells have been applied and to generate orientations with known distribution Roberts approach has been used. For such a model elastic modules for discrete sets of grains with known volumes and orientations from one hand and with known ODFs from the other hand were computed. It has been found that both these approaches lead to the same values for the elastic modules, when a number of grains tend to infinity. The number of grains for which the valuable difference between the results of calculations with and without taking grain area distribution into account is less than 8000 for cubic symmetry and 10000 for hexagonal symmetry.

The investigation has been performed at the Frank Laboratory of Neutron Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna, 2002

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ЛР № 020579 от 23.06.97.
Подписано в печать 11.04.2002.
Формат 60 × 90/16. Бумага офсетная. Печать офсетная.
Усл. печ. л. 1,18. Уч.-изд. л. 1,62. Тираж 290 экз. Заказ № 53225.

Издательский отдел Объединенного института ядерных исследований
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