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Relations between grain boundary character distribution, misorientation distribution and two-point orientation distribution

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ABSTRACT

Relations are found between grain boundary character distribution, misorientation distribution and two-point orientation distribution. Some of these relations are analogies for polycrystals of the Debye–Anderson–Brumberger formula and Berryman formula established for two-phase composites.

1. Introduction

Quantitative characterization of random microstructures is a fundamental open problem in theory of materials. There are two approaches to describe random microstructures. One is to introduce explicitly the ensemble of admissible microgeometries and prescribe probabilistic measure on this ensemble. For example, matrix with spherical inclusions can be viewed as an ensemble of non-overlapping spheres. The simplest probabilistic measure on this ensemble is introduced by the assumption that all positions of spheres are equiprobable. Another approach employs theory of random fields. In this approach material characteristics are viewed as random fields. To specify a random field one has to know n-point probability densities for all n ranging from 1 to infinity (see, e.g., Rytov, Kravtsov, & Tatarskii, 1989). There are exceptional random fields, like Gaussian fields, for which the entire infinite chain of n-point probability densities is specified by a few functions, but in a generic case a complete description of random microstructures requires the knowledge of an infinite number of functions. This is not possible, and the usual description employs only a few probability densities, typically one-point and two-point probability densities.

Each of the two approaches has its own advantages. In the first approach, it is easy to figure out the role of geometrical parameters of microstructures. In the second approach, it is easy to link the probability densities to physical characteristics. One of the basic open questions is: what are the relationships between the two approaches? Another version of this question: how do the geometrical parameters of microstructures affect probability densities? For one-point probability densities the answer is simple. For example, one-point probability density of materials characteristics in multi-phase composites is a function of phase concentrations. In contrast, the relations between two-point probability densities and geometrical parameters are non-trivial and rarely known. An important result of this kind was found by Debye, Anderson and Brumberger (Debye et al., 1957). They

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considered the correlation function $h_0(\tau)$ of porous materials. Function $h_0(\tau)$ has the following meaning: if one casts vector τ onto microstructure randomly, then $1 - h_0(\tau)$ is the probability that the starting point of the vector τ is in the matrix, while the end point is in a pore. Debye, Anderson and Brumberger found that $h_0(\tau)$ is simply related to the specific interphase area γ (interphase area per unit volume),

$$h_0(\tau) \sim 1 - \gamma|\tau|/4c_1c_2 \quad \text{as } |\tau| \to 0. \tag{1}$$

Here $|\tau|$ is the length of vector τ, c_1 and c_2 are phase concentrations $(c_1 + c_2 = 1)$. In fact, formula (1) holds for any two-phase material. As follows from (1), $\tau = 0$ is a singular point of the correlation function: derivatives of $h_0(\tau)$ have different limits along different paths going to the point $\tau = 0$, while second derivatives tend to infinity as $\tau \to 0$. The asymptotics of $h_0(\tau)$ at $\tau = 0$ determine the asymptotics of the Fourier transform of $h_0(\tau)$ at large wave numbers. The Fourier transform of $h_0(\tau)$ can be found experimentally from the scatter of electro-magnetic waves. This gives a method for estimation of specific interphase area by means of (1). Function $h_0(\tau)$ is called the Debye X-ray correlation function in the physics literature.

Formula (1) was established for isotropic composites. For such composites $h_0(\tau)$ depends on τ only through $|\tau|$. Berryman (1987) obtained a generalization of (1) for anisotropic two-phase composites. This generalization can be written as

$$\left\langle h_0\left(\varepsilon\overrightarrow{\xi}\right)\right\rangle_{\overrightarrow{\xi}} \sim 1 - \gamma\varepsilon/4c_1c_2 \quad \text{as } \varepsilon \to 0 \tag{2}$$

where $\langle\cdot\rangle_{\overrightarrow{\xi}}$ means average value over all unit vectors $\overrightarrow{\xi}$ homogeneously distributed over unit sphere.

The next order terms in the expansion of $h_0(\tau)$ in the vicinity of zero contain more subtle parameters of microgeometry, like curvatures of the interphase surfaces and the number of nearest neighbors (Frisch & Stillinger, 1963). Note also the results for two-point probability densities in composites with spherical inclusions reviewed by Torquato (2002) and the relations between 2D cross section statistics and 3D statistics (Berryman, 1998).

This paper aims to establish the relations similar to (1), (2) for polycrystals. It turns out that these are the relations linking grain boundary character distribution (GBCD), misorientation distribution and two-point orientation distribution. The major motivation for this work was the need for such relations in the study of probabilistic characteristics of local fields (currents, stresses) in polycrystals (Berdichevsky, 2009, 2015). Note that GBCD affects many processes in polycrystals (Bange, 1994; Kim, Rollet, & Rohrer, 2006; Saylor, El Dasher, Rollet, & Rohrer, 2004; Watanabe, 1992). Two-point orientation distributions were studied experimentally by Gao, Przybyla, and Adams (2006).

We begin with the necessary definitions (Sections 2 and 3), in Section 4 the relations between orientation distributions are derived, and in Section 5 some consequences of these relations are discussed.

2. Bulk orientation distributions

We consider characteristics of polycrystals, which do not depend on the sample size. So, by polycrystal we mean a random tesselation of three-dimensional space into grains. In each grain an orthogonal frame is given. Each frame can be obtained by rotation of some observer's frame, and, thus, specified by three rotation parameters. As such we will use Euler angles $\varphi = \{\varphi_1, \phi, \varphi_2\}$, $0 \le \varphi_1 \le 2\pi$, $0 \le \phi \le \pi$, $0 \le \varphi_2 \le 2\pi$. Angles φ are constant in each grain, and $\varphi(x)$ is a piece-wise constant function. We consider an ensemble of polycrystals, i.e. an ensemble consisting on various tesselations of space in grains and various distributions of angles over grains. The members of the ensembles are marked by the symbol ω, and the set of all ω is denoted by Ω. So, angles φ are functions of two variables, x and ω: $\varphi = \varphi(x, \omega)$. Some probabilistic measure is given on Ω. Mathematical expectation is integration over Ω with probabilistic measure, it is denoted by the symbol M. One can introduce one-point and two-point probability densities of $\varphi(x, \omega)$ as

$$f_1(x, \varphi) = M\delta(\varphi - \varphi(x, \omega)),$$
$$f_2\left(x, \varphi; x', \varphi'\right) = M\delta(\varphi - \varphi(x, \omega))\delta\left(\varphi' - \varphi\left(x', \omega\right)\right).$$

Here $\delta(\varphi)$ is δ–function in three-dimensional space of Euler angles, i.e. the product of three one-dimensional δ-functions, $\delta(\varphi) \equiv \delta(\varphi_1)\delta(\phi)\delta(\varphi_2)$. Following tradition, we will call f_1 and f_2 one-point and two-point orientation distributions. Random field $\varphi(x, \omega)$ is assumed to be stationary. This means that the probabilistic measure is invariant with respect to space shifts. In particular, one-point and two-point orientation distributions are invariant with respect to space shifts. Thus, one-point orientation distribution depends only on φ, $f_1 = f(\varphi)$, and two-point orientation density depends on x and x' only through the difference $\tau = x' - x$: $f_2 = f\left(\varphi; \tau, \varphi'\right)$. We assume also that random field is ergodic. This means that mathematical expectation of any function of $\varphi(x, \omega)$ coincides with the space average $\langle \cdot \rangle$. For any function $\alpha(x)$ the space average is, by definition, the limit

$$\langle\alpha(x)\rangle = \lim_{|V|\to\infty} \frac{1}{|V|}\int_V \alpha(x)dV,$$

$|V|$ being the volume of ball V. Accordingly, one-point and two-point orientation distributions can be defined also as

$$f(\varphi) = \langle\delta(\varphi - \varphi(x, \omega))\rangle \tag{3}$$
$$f\left(\varphi; \tau, \varphi'\right) = \left\langle\delta(\varphi - \varphi(x, \omega))\delta\left(\varphi' - \varphi(x + \tau, \omega)\right)\right\rangle$$