Characterization of chaos in polycrystal/foam microstructures and related issues

V. L. Berdichevsky,

Mechanical Engineering, Wayne State University, Detroit, MI 48202, USA

To characterize a material with random microstructure using the language of probability theory, one has to prescribe an infinite sequence of multi-point probability density functions. In experiments one can hardly go beyond one-point and two-point probability densities. In case of polycrystals, this yields the following difficulty: the one-point and two-point probability densities determined for a given polycrystal describe not only this particular microsctructure but many other microgeometries that are quite different from the polycrystal microgeometry. Thus, an alternative and more adequate language is needed. In this paper such a language is suggested. It is based on the solution of the following auxiliary problem which is of independent interest. Let a set of bounded regions of three-dimensional space, grains, be given. The grains can be translated and rotated as rigid bodies. What are the necessary and sufficient conditions that, after an appropriate motion, the grains form a polycrystal, i.e. fit each other without gaps and overlapping, or, in other words, form a tessellation of space? Such necessary and sufficient conditions (tessellation conditions) are obtained and form the technical ground for other results of the paper. The tessellation conditions yield an infinite chain of constraints on characteristics of grain geometry (such as volumes, centers of gravity, moments of inertia, etc). The constraints select a manifold in the phase space of all microstructures. Probability measures that involve only geometrical parameters of grains are introduced as probability measures on this manifold. Several issues have been addressed using these new probabilistic characteristics:

Most chaotic polycrystal/foam microstructures. According to Laplace's principle of insufficient reasoning, such are equiprobable microstructures. The probability distributions of grain characteristics are found for the most chaotic microstructures in the leading approximation.

Grain growth. The experimental grain size distribution in self-similar grain growth is compared with the most chaotic grain size distribution. These two distributions turn out to be practically identical. This indicates that the process of grain growth results in development of the most chaotic microstructures.

Dynamics of grain growth. The idea that chaos in grain growth increases and, when the grain growth reaches the self-similar regime, the microstructures become most chaotic, is taken as a "first principle" in construction of the dynamic equation for probability density of grain sizes. Remarkably, such "first principle" determines the equation for probability density almost uniquely. This equation admits analytical investigation and supports an earlier conjecture (Berdichevsky 2008) that entropy of microstructure decays in isolated systems (entropy per one grain grows as chaos increases, while total entropy, which is the product of entropy per one grain and the number of grains, decays because the number of grains decays faster than entropy per one grain grows).

Bounds for effective moduli: Hashin-Shtrikman bounds do not work, if the polycrystal microstructure is not statistically isotropic. Statistically anisotropic microstructures are quite common. An important example is the microstructure of rolled metal sheets. The bounds for statistically anisotropic polycrystals are obtained in terms of statistical characteristics of the grain geometry.

Local stress fields. Usually, local stress fields can be found in random structures only by numerical simulations. It is highly desirable to develop an approach allowing one to find the probabilistic characteristics of local stress fields directly from the knowledge of the probabilistic characteristics of grain misorientations. This is important for determining texture evolution, plastic deformation, fatigue, etc. A variational principle for probabilistic measures of local stress field was suggested by the author some time ago (Berdichevsky, J. Appl. Math. Mech. (PMM), 1987, Berdichevsky, Variational principles of continuum mechanics, Springer, 2009, Sect. 18.2-18.3). In this paper, this variational principle is applied to determine the probabilistic characteristics of local stress fields when the information on the polycrystal microstructure is given in terms of probabilistic characteristics of the grain geometry. Most attention is paid to rolled metals, for which Hashin-Shtrikman local fields do not provide a good approximation. The general equations and some exact solution are obtained.