An information-theoretic approach for obtaining property PDFs from macro specifications of microstructural variability

Nicholas Zabaras, Veera Sundararaghavan and Sethuraman Sankaran

Materials Process Design and Control Laboratory, Sibley School of Mechanical and Aerospace Engineering
188 Frank H.T. Rhodes Hall, Cornell University, Ithaca, NY 14853-3801, USA

Abstract

Probability distribution functions (PDFs) providing a complete representation of property variability in polycrystalline materials are difficult to obtain. Reconstruction of a PDF of a material property based on limited microstructural information is an inverse problem of practical significance since many macroscopic properties depend strongly on geometrical variability of the micro-constituents. We characterize the unknown probabilities of the microstructural parameters of polycrystalline alloys making use of average values (and lower moments) of grain sizes, average orientation distribution functions (ODFs) and using the concepts of maximum information entropy (MaxEnt) and stochastic geometry.

Introduction

All materials comprise of various length scales emphasizing the different resolution levels at which practical components may be viewed. The physical basis of a material's mechanical response stems from lower scales. A particular problem of interest addressed here is the determination of effective behavior of polycrystalline materials based on uncertainties induced due to random nature of microstructures. The fundamental reason behind this uncertainty is due to the fact that microstructual images can be obtained only at a limited number of material points on a sample (a material point is a distinct point on the macro scale and has a microstructure associated with it). The information that is obtained from this limited set is not sufficient to deterministically characterize the microstructures that are present in the specimen. In our formalism, microstructures are considered as realizations of a random field. We utilize the principle of MaxEnt to find the distribution of microstructures that satisfy the measured information about the microstructure. The reconstructed microstructures are interrogated to obtain statistics of their homogenized plastic properties. This procedure is summarized in Fig. 1 for the case of estimating plastic properties of two-dimensional Al microstructures using grain size and orientation distribution functions.

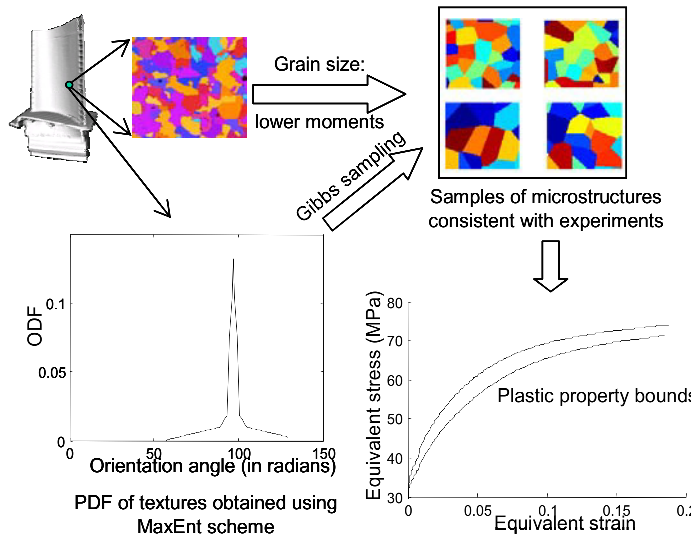

Figure 1: Experimental samples of microstructure are obtained using x-ray measurements. Reconstruction is based on two features, namely the grain size, and ODF. Both are treated as random fields, whose PDF are obtained using the MaxEnt scheme. Microstructure samples are generated using voronoi tessellations and grains are randomly assigned orientations based on a PDF of ODFs. The resulting microstructures are interrogated using [1] and the bounds of plastic properties are obtained.

The principle of maximum entropy (MaxEnt)

Suppose that we have insufficient knowledge about an entity. The MaxEnt approach provides a rationale to obtain the entire probabilistic variability about the entity [2][3]. Since the problem of obtaining a distribution of microstructures using average information about microstructural features is ill posed, we pose an additional requirement that the entropy of the distribution of the microstructures is maximized. It is to be noted that the entropy function is convex [4] and in an unconstrained problem, it achieves the maximum when all the possible events are equiprobable. This means that when we do not have any information about a system, the most unbiased prediction about the behavior of the system is by assuming that all possible outcomes are equiprobable. The knowledge about microstructures obtained from experimental measurements is posed as a constraint. The distribution that is obtained using MaxEnt is the most uniform distribution satisfying the given constraints. For details of mathematical techniques used in entropy optimization, refer [5][6][7][8].

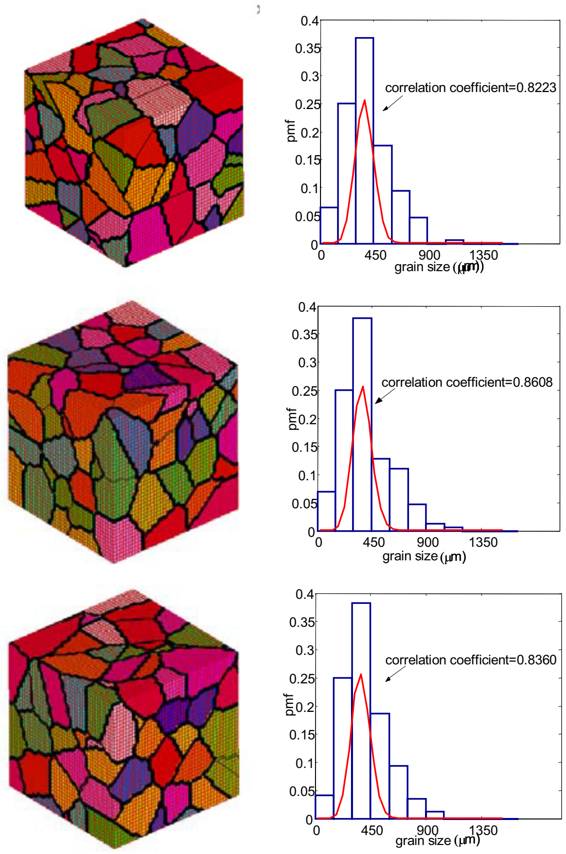

Figure 2: The figure shows reconstructed microstructures and the comparison of their grain size distribution with MaxEnt grain size distribution.

Reconstruction of 3D microstructures

The problem of reconstruction of 3D microstructures comprises of the following sub-problems: (i) representation of 3D microstructures (ii) reconstructing microstructures that satisfy observable information about their features (iii) obtaining the homogenized non-linear properties of the microstructures such as plastic stress-strain curves. The voronoi cell tessellation technique [9][10][11][12] is employed for representing the microstructures. A set of polyhedra are used to represent the 3D space comprising of the microstructures. The polyhedra themselves are chosen so that their grain size distribution matches the PDF of grain sizes obtained using the MaxEnt principle. Since the task of exactly constructing voronoi tessellations of the given grain size distribution is intractable, a simpler version of the problem is chosen. A Monte Carlo scheme is utilized whereby a large database of microstructures is created using voronoi tessellations and those microstructures which have a correlation coefficient ($R_{corr}>0.8$) are accepted. Figure 2 shows some microstructures which were constructed using the above-mentioned scheme. All grains are assigned orientations based on a distribution of ODF's reconstructed from average ODF measurements. This PDF is obtained using the MaxEnt scheme and samples of reconstructed ODFs are shown in Fig. 3 using the Rodrigues-Frank representation. Each of these microstructures are interrogated using the homogenization method provided in [1]. The equivalent stress-strain curves are plotted for these samples. The MaxEnt technique not only provides the extreme values of the stress-strain response but also PDFs of the response, which is useful in stochastic simulations.

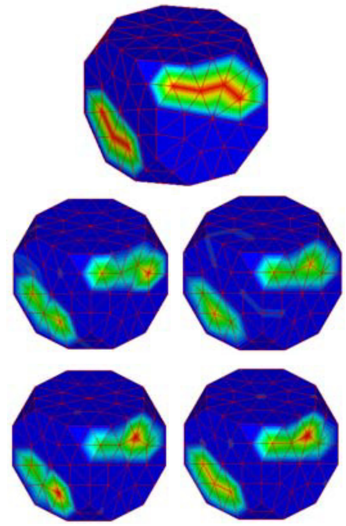

Figure 3: The figure shows reconstructed samples of ODF's based on the given ODF which is shown on top.

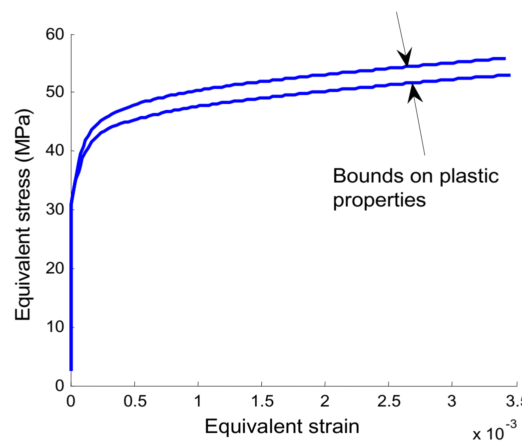

Figure 4: The figure shows bounds of the plastic properties obtained using the reconstructed microstructural samples and employing homogenization techniques.

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