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Thermal Response Variability of Random Polycrystalline Microstructures

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Abstract. A data-driven model reduction strategy is presented for the representation of random polycrystal microstructures. Given a set of microstructure snapshots that satisfy certain statistical constraints such as given low-order moments of the grain size distribution, using a non-linear manifold learning approach, we identify the intrinsic low-dimensionality of the microstructure manifold. In addition to grain size, a linear dimensionality reduction technique (Karhunun-Loéve Expansion) is used to reduce the texture representation. The space of viable microstructures is mapped to a low-dimensional region thus facilitating the analysis and design of polycrystal microstructures. This methodology allows us to sample microstructure features in the reduced-order space thus making it a highly efficient, low-dimensional surrogate for representing microstructures (grain size and texture). We demonstrate the model reduction approach by computing the variability of homogenized thermal properties using sparse grid collocation in the reduced-order space that describes the grain size and orientation variability.

AMS subject classifications: 52B10, 65D18, 68U05, 68U07

Key words: Non-linear model reduction, polycrystalline microstructure, homogenization, microstructure reconstruction, stochastic analysis, Karhunun-Loéve Expansion, multiscale modeling, heat conduction.

1 Introduction

Mathematical representation of microstructures is essential in many tasks including the exploration of the process/structure/property triangle [1] and optimizing microstruc-

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tural topology for achieving optimal properties [2]. In this paper, we are interested in exploring the variability of homogenized thermal properties of microstructures induced by the random nature of the microstructure topology. Computing error-bars of materials properties induced by microstructural uncertainty was examined earlier in [3, 4] using Maximum Entropy methods. The microstructure uncertainty can be introduced in many ways. Here, we assume that we are given a finite set of microstructure snapshots that share some common features, usually in terms of low-order statistical moments of grain size and texture. With this data, we are interested to build a probabilistic model of the underlying random microstructures that share these given statistical features. To efficiently utilize this large scale experimental data, it is important to efficiently compress the data into low-dimensional models.

A polycrystalline microstructure is herein described by its grain size and texture. We are interested in *constructing reduced-order representations of polycrystalline microstructure based on available experimental or simulation-based data* (microstructural snapshots). Given a set of microstructures having the same constituent elements and the same processing history, each microstructure will satisfy some statistical correlations that inherently define its material distribution (volume fraction of one constituent element) and/or the processing history (a specific grain size distribution and/or preferred texture). A reduced-order model that satisfies these statistical correlations while efficiently encoding and quantifying the variations in this data set would significantly accelerate and simplify analysis.

In [5], a (linear) model reduction scheme based on Principle Component Analysis (PCA) was developed for two-phase composite microstructures. However, polycrystalline microstructures contain nonlinear structures that are not captured by PCA. In [6], a nonlinear dimensionality reduction (NLDR) strategy was proposed to embed data variations into a low-dimensional manifold. This methodology was used to construct a reduced-order model of homogenized thermal diffusivity of a two-phase microstructure. Our emphasis here is to extend this NLDR methodology to develop a low-dimensional representation of *polycrystalline microstructures defined in terms of their grain size and texture distribution*. This problem poses significant challenges: (a) reconstruction of microstructures from the low-dimensional space is a difficult task in essence requiring interpolation from the neighboring microstructures while at the same time satisfying all given manifold properties, and (b) NLDR requires a notion of distance between microstructures [6].

Besides the grain size distribution, material properties of polycrystalline microstructures are also highly-dependent on texture. Rodrigues parametrization is often used to describe the orientations of grains. This axis-angle parametrization is convenient when certain symmetries are known in the crystal [7] and therefore a fundamental zone in Rodrigues space exists (e.g., cubic, hcp crystals). The Orientation Distribution Function (ODF) defined in Rodrigues space was used in our earlier work to represent texture [8–10]. If no prescribed information is provided, the orientation of a grain can be totally random. In reality, materials acquire certain preferred texture after processing. This introduces correlations among grain orientations and enable us to perform model reduction techniques on the texture. Some linear approaches have shown success in re-