Acta Materialia 129 (2017) 428–438

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Reduced-order structure-property linkages for polycrystalline microstructures based on 2-point statistics

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ARTICLE INFO

Article history:
Received 30 November 2016
Received in revised form
26 February 2017
Accepted 6 March 2017
Available online 8 March 2017

Keywords:
2-Point correlations
Microstructure
Computational model
Crystal plasticity
Reduced-order model

ABSTRACT

Computationally efficient structure-property (S-P) linkages (i.e., reduced order models) are a necessary key ingredient in accelerating the rate of development and deployment of structural materials. This need represents a major challenge for polycrystalline materials, which exhibit rich heterogeneous microstructure at multiple structure/length scales, and exhibit a wide range of properties. In this study, a novel framework is described for extracting S-P linkages in polycrystalline microstructures that are obtained using 2-point spatial correlations (also called 2-point statistics) to quantify the material's microstructure, and principal component analysis (PCA) to represent this information in a reduced dimensional space. Additionally, it is demonstrated that the use of generalized spherical harmonics (GSH) as a Fourier basis for functions defined on the orientation space leads to a compact and computationally efficient representation of the desired S-P linkages. In this study, these novel protocols are developed and demonstrated for elastic stiffness and yield strength predictions for $\alpha-$ Ti microstructures using a dataset produced through microscale finite element simulations.

1. Introduction

Materials development and deployment efforts require evaluation of the properties of large sets of potential material internal structures (generically referred to as microstructures; this description also includes information regarding chemical composition at the relevant length scales) [1–13]. Currently, experiments and simulations are used for such analyses at a high cost, severely limiting the extent of the materials design spaces explored [14,15]. In addition, most of the current approaches (e.g., finite element models) employed in modeling and simulation are not readily invertible, i.e., it isn't easy to determine a candidate microstructure given a set of desired properties. Reduced order models are critical to the acceleration of materials discovery and development, as they enable high throughput exploration of the materials design spaces for rapid down selection [1,6,7,16–18]. In this work, we specifically focus on reduced order structure-property (S-P) linkages for polycrystalline microstructures that exhibit rich heterogeneity in the spatial distribution of the crystal lattice orientation at the mesoscale (also referred to as grain-scale). These microstructures exhibit strongly anisotropic elastic and inelastic properties at the macroscale [5,16,19–31].

It is important to pursue the development of reduced order models within the context of established physically-based theories. There is indeed a rich literature on homogenization theories for polycrystalline microstructures that can be used to guide the development of surrogate models. For elastic stiffness or compliance components, the foundational concepts can be traced back to the elementary bounds established by Voigt [32], Reuss [33], and Hill [34], as well as the more sophisticated self-consistent approaches of Kroner [35], which leverage Eshelby's solution [36]. For inelastic properties, analogous foundations can be traced to the works of Taylor [37] and Sachs [38]. Detailed discussion of these theories cast in a modern continuum mechanics framework can be found in Nemat-Nasser and Mori [39], Milton [40], Mura [41], Qu and Cherkaoui [42] and Roters [43].

The central limitation of the theories mentioned above is that

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http://dx.doi.org/10.1016/j.actamat.2017.03.009
1359-6454/

they can only incorporate a very limited amount of information regarding the material microstructure. To date, microstructural information included in the application of established composite theories to polycrystalline microstructures has largely been limited to the orientation distribution (also called texture) in the sample, and in some cases, averaged shape factors (based on idealizing the grains as ellipsoids) [31,44]. The main exception to these statements comes in the form of statistical continuum theories formulated originally by Brown [45] for electrical properties of materials, and subsequently introduced by Volkov and Klinskikh [46], Lomakin [47], and Beran and Molyneux [48] for mechanical properties. These ideas have been further refined in later years by Beran [49,50], Kröner [51–53], Torquato [54–56], Adams [16,57,58], and others [59–63]. A unique feature of this formulation is that the effective property is expressed as a series expansion, where each term represents a contribution of a specific microstructural attribute expressed in the formalism of n-point statistics [57,58,64,65]. In some cases, the pre-factor for each term in the series can be evaluated using known Green's functions [16,59]. Most importantly, this approach allows one to include as much detail of the material microstructure as one wishes in arriving at the homogenized properties of interest.

The sophisticated higher-order homogenization theories mentioned above have encountered some difficulties in their implementation. First, the Green's functions required for the implementation of these theories are only available for a limited number of physical phenomena. Second, the convergence of the series is rather slow for high contrast composites [54,64]. Over the past decade, Kalidindi and coworkers [1,16,19,66–76] have developed a novel data science approach that still utilizes the basic mathematical formulation of the statistical continuum theories, and circumvents the central impediments mentioned above by employing modern data science tools. Mainly, it has been shown that the elusive pre-factors (related to Green's functions) in the series expansion can be calibrated to results from numerical simulations (e.g., performed using finite element models). This new framework for establishing S-P linkages has been referred as materials knowledge systems (MKS) and has addressed both homogenization (bottom-up) [68,70,73,74] and localization (top-down) problems [19,66,67,69,71,72,75,76]. It is clarified here that the term "MKS framework" in our prior work was used exclusively with the latter linkages. However, since both the homogenization and localization linkages developed in this new data science framework share the same foundations (they both come from the same statistical continuum theories discussed earlier), we will henceforth refer to both homogenization and localization linkages established using this approach as MKS linkages.

In the MKS framework, the homogenization S-P linkages (reduced-order models) [1,68,70,73,74] connect the microstructure descriptors (inputs) to the effective macroscale properties (outputs). These linkages are typically expressed in the form of a polynomial series. The input microstructure descriptors are generally based on principal component analysis (PCA) [77] of the 2-point spatial correlations obtained from all the microstructures in the ensemble studied. The outputs have frequently included elastic stiffness or compliance components and the yield strength. Much of the prior work has been limited to materials with multiple distinct phases [1,68,70,73,74].

The main goal of this work is to extend the MKS homogenization framework to polycrystalline microstructures, where the local material state in each voxel is characterized by a crystal lattice orientation (defined by an ordered set of three Euler angles). Prior attempts [78,79] in this direction have binned the local state space (i.e., the orientation space) and treated the material as a composite; each bin in the orientation space corresponded to a distinct local state. However, this approach requires a very large number of orientation bins in order to obtain a representation of satisfactory fidelity. In this work, we will develop an extension to the existing MKS framework for homogenization S-P linkages by using generalized spherical harmonics (GSH) [80] for the functional components over the orientation space. We will specifically demonstrate that this approach produces computationally efficient, highly compact representations of reduced-order S-P linkages for polycrystalline microstructures. Note that GSH have already been used successfully in related problems [19,29,57,81,82], including certain MKS localization linkages [19,66,69]. The efficiency and efficacy of the new approach developed and presented in this work is specifically demonstrated through the predictions of the elastic stiffness and yield strengths in a variety of α-titanium microstructures. It is emphasized that S-P linkages can only attempt to match the physics of whatever process was used to produce the set of calibration data. Consequently, the linkages in this work are calibrated using the results of CPFE simulations on synthetic microstructures, and the success of this approach is evaluated by comparing against results of that same model.

2. Current theoretical framework

In order to construct S-P linkages, microstructural information must be presented in a form that allows for a rigorous quantitative comparison. Unfortunately, images of microstructure cannot fulfill this role in their raw representations. In other words, a pixel by pixel comparison of two random microstructures, either from the same sample or from different samples, will not reveal useful information. Traditionally, metrics such as grain size distributions and phase volume fractions have been used to capture the salient microstructural information [83,84]. However, these approaches do not consider the complexities of the microstructure geometry with sufficient fidelity for many properties of interest. In recent years, Kalidindi and co-workers have employed 2-point spatial correlations to evaluate microstructural distances [64], cluster microstructures [74,85], and to provide a basis for the construction of S-P linkages [68,70,73]. This higher order statistical representation of microstructure precludes the need to manually select microstructure features (and potentially introduce bias) in the construction of S-P linkages; the 2-point spatial correlations already include many of the conventionally defined metrics of the microstructure.

Following the framework developed by Adams et al. [5,16,57], the microstructure in hierarchical materials systems can be mathematically captured through the function $m(h,\boldsymbol{x})$, which reflects the probability density of finding local state h (within an incremental Δh around h) at the spatial location $\boldsymbol{x}$. In this formalism, h and $\boldsymbol{x}$ are both treated as continuous variables. However, in practice it is much more useful to employ a discretized description of the microstructure function. Moreover, most experimental characterization techniques recover only a discretized description of the microstructure (as a consequence of the resolution limits of the equipment). Recognizing this, Adams et al. [5,16,57] have proposed a discretized description of the microstructure function $M_{\boldsymbol{s}}^{n}$ based on primitive binning of both the spatial domain and the local state space, i.e.,

$$m(h,\boldsymbol{x})\Delta h \approx \sum_{n=1}^{N}\sum_{\boldsymbol{s}=1}^{\boldsymbol{S}} M_{\boldsymbol{s}}^{n}\chi_{n}(h)\chi_{\boldsymbol{s}}(\boldsymbol{x}) \tag{1}$$

where the indicator function $\chi_i(\,)$ is defined such that it is equal to one if and only if the argument belongs to the bin labeled i and zero otherwise, and Δh denotes the size of the local state bin employed. An important consequence of this definition is that $M_{\boldsymbol{s}}^{n}$ has a very