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ScienceDirect

Acta Materialia 81 (2014) 151–160

Acta MATERIALIA

www.elsevier.com/locate/actamat

Calibrated localization relationships for elastic response of polycrystalline aggregates

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Received 30 June 2014; received in revised form 8 August 2014; accepted 11 August 2014
Available online 7 September 2014

Abstract

In recent years, our research group has formulated a new framework called materials knowledge systems (MKS) for establishing highly accurate reduced-order (surrogate) models for localization (opposite of homogenization) linkages in hierarchical materials systems. These new computationally efficient linkages are designed to capture accurately the microscale spatial distribution of a response field of interest in the representative volume element (RVE) of a material, when subjected to an imposed macroscale loading condition. In prior work, the viability and computational advantages of the MKS approach were demonstrated in a number of case studies involving multiphase composites, where the local material state in each spatial bin of the RVE was permitted to be any one of a limited number of material phases (i.e. restricted to a set of discrete local states of the material). In this paper, we present a major extension to the MKS framework that allows a computationally efficient treatment of a significantly more complex local state of the material, i.e. crystal lattice orientation. This extension of the MKS framework is formulated by the use of suitable Fourier representation of the influence functions. This paper describes this new formulation and the associated calibration protocols, and demonstrates its viability with case studies comprising low and moderate contrast cubic and hexagonal polycrystals.

Keywords: Materials knowledge systems; Localization; Polycrystal; Generalized spherical harmonics; Multi-scale modeling

1. Introduction

Virtually all materials of interest to emerging advanced technologies exhibit complex hierarchical internal structures (hereafter generically referred to as microstructures). The successful design and manufacture of new/improved materials with vastly enhanced properties or performance characteristics are contingent on the availability of a computational framework that efficiently bridges the relevant hierarchical length/structure scales in the material (also referred to as hierarchical multiscaling) [1–5]. In most hierarchical multiscaling approaches, the focus has thus far been in communicating the effective properties to the higher length scales, i.e. on homogenization. There is often very little information passed in the opposite direction, i.e. localization. As an example, localization may involve the spatial distribution of the response field of interest (e.g. stress or strain rate fields) at the microscale (on a representative volume element) for an imposed loading condition at the macroscale.

In recent years, our research group has formulated a novel, computationally efficient, bi-directional, scale-bridging framework called materials knowledge systems (MKS) [6–11]. In the MKS framework, the focus is on expressing the localization relationships of interest in the form of a simple algebraic series whose terms capture systematically the individual contributions from a hierarchy of local microstructure descriptors. The specific form of the algebraic series used in the MKS approach is adopted from

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http://dx.doi.org/10.1016/j.actamat.2014.08.022
1359-6454/

the well-established statistical continuum theories [12–16]. In both of these approaches (MKS and the statistical continuum theories), the localization linkage takes the form of a series where each term is expressed as a convolution product of a physics-capturing kernel with a higher-order local microstructure descriptor. However, the main difference between the two approaches is that the localization linkage in the MKS approach is calibrated to datasets obtained from established numerical approaches for the materials phenomena of interest. For example, in studies of micromechanical phenomena, the physics-capturing kernels in the MKS linkages are calibrated to results obtained from finite element models for a diverse set of example microstructures. The most impressive benefit of the MKS approach lies in the dramatic reduction of the computational cost, often by several orders of magnitude compared to numerical approaches typically employed in microstructure design problems. The MKS methodology has thus far been successfully applied to capturing thermo-elastic stress (or strain) distributions in composite representative volume elements (RVEs), rigid-viscoplastic strain rate fields in composite RVEs and the evolution of the composition fields in the spinodal decomposition of binary alloys [7,8,10].

Whilst MKS has enjoyed several remarkable successes thus far, it is still in its early stages of development. Almost all of the case studies explored thus far have been restricted to composite material systems with a limited set of discrete local material states (i.e. two-phase or three-phase microstructures). However, most materials of interest in emerging technologies exhibit local states that are much more complicated. For example, most advanced structural materials exhibit polycrystalline microstructures, where the spatial distribution of the crystal lattice orientations at the microscale plays an important role in controlling their effective properties. High throughput evaluation of the responses of a large set of microstructures (as one might need in optimizing the material performance in a selected application) with such complex local states requires a major extension of the MKS framework that allows efficient treatment of tensorial local states (e.g. crystal lattice orientation) and their associated continuous local state spaces. In this regard, it should be recognized that it is possible to treat continuous local states simply by binning the continuous local state space (as described in our earlier work [7]). However, a primitive binning of the local state space is expected to prove highly inefficient, computationally, in capturing accurately the localization linkages of interest, especially in situations where the microscale response in the material microstructure shows high sensitivity to the local state (e.g. plastic response of crystalline states).

This paper presents the needed extension to the theoretical framework of the MKS approach to allow a rigorous treatment of the crystal lattice orientation as the local state variable. This is accomplished through the use of generalized spherical harmonics (GSHs) [17] for capturing the orientation dependence of the influence kernels in the MKS linkages. It should be noted that GSHs have already been demonstrated to produce highly efficient and compact spectral descriptions of functions defined on the orientation space in other applications in prior literature [2,11,18–32]. The viability of the new MKS formulation developed in this work is demonstrated with case studies on selected cubic and hexagonal polycrystalline material systems.

2. Review of MKS framework

The MKS framework is built on a digital description of the microstructure, where the spatial domain of the microstructure (presumably identifying a representative volume) and the corresponding local state space (the set of all possible local states that may be encountered in the microstructure) are both uniformly binned using suitable invariant measures [33]. Let $s = 1, 2, \ldots, S$ enumerate the spatial bins (or voxels) in the microscale volume of interest. Similarly, let $h = 1, 2, \ldots, H$ enumerate the local states of interest in a multiphase composite material system. With this notation, the digital representation of the microstructure function, denoted as m_s^h, reflects the volume fraction of local states identified by h in the spatial bin s. Digital representations of the microstructure function described here have already been successfully employed in many applications, including the fast computation of microstructure metrics and variance [2,34,35], automated identification of salient microstructure features in large datasets [2,36], determination of representative volume elements from an ensemble of datasets [37–40], microstructure reconstructions based on statistical correlation functions [16,41–44] and the establishment of processing–structure–property linkages [7–11,15,19,20,45–50].

The form of the localization relationships in the MKS framework is adopted from Kroner's statistical continuum theories [12,13,16] and can be expressed as [7–9,11,49]:

$$\boldsymbol{p}_s = \left(\sum_{h=1}^{H} \sum_{t=1}^{S} \boldsymbol{\alpha}_t^h \, m_{s+t}^h + \sum_{h=1}^{H} \sum_{h'=1}^{H} \sum_{t=1}^{S} \sum_{t'=1}^{S} \boldsymbol{\alpha}_{tt'}^{hh'} \, m_{s+t}^h m_{s+t+t'}^{h'} + \cdots \right) \langle \boldsymbol{p} \rangle \tag{1}$$

where $\boldsymbol{p}_s$ denotes the local response in the spatial cell of interest s and $\langle \boldsymbol{p} \rangle$ represents the corresponding macroscopic quantity (imposed at the macroscale). It is noted that all of the MKS formulations to date have been designed such that $\langle \boldsymbol{p} \rangle$ is indeed the volume average of the $\boldsymbol{p}_s$ over the entire spatial domain of the microstructure. In other words, the localization linkages in the MKS formulation are aimed at capturing the spatial distribution of the quantity imposed at the higher length scale (i.e. $\langle \boldsymbol{p} \rangle$) to the lower length scale (i.e. $\boldsymbol{p}_s$), while conserving the overall amount. In Eq. (1), $\boldsymbol{\alpha}_t^h$ and $\boldsymbol{\alpha}_{tt'}^{hh'}$ are referred to as the first-order and second-order influence coefficients, respectively, and denote the physics-capturing kernels. First-order influence coefficients, $\boldsymbol{\alpha}_t^h$, capture the influence of local state h in spatial cell separated by a vector t from spatial cell s. Likewise,