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Computational homogenization and micromechanical analysis of textured polycrystalline materials

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Highlights

- Computational methodology for the analysis of textured polycrystalline materials.
- Analysis of bulk properties and detailed microstructural stress distributions.
- Applicable to real microstructures obtained from electron backscatter diffraction.
- Results compared with Voigt, Reuss, Voigt–Reuss–Hill and self-consistent estimates.
- Software toolbox has been developed for the analysis of real polycrystalline materials.

Abstract

We present a numerical methodology for the thermomechanical analysis of real polycrystalline material microstructures obtained using electron backscatter diffraction techniques. The asymptotic expansion homogenization method is used in conjunction with the finite element method to perform comprehensive micromechanical analyses and determine the effective thermoelastic properties of polycrystalline materials. Smooth grain boundaries are generated from the discretely sampled electron backscatter diffraction data of real polycrystalline materials. The microscale displacements, strains and stresses are related to the macroscale temperature change and strains through 21 distinct characteristic functions. The three-dimensional equilibrium equations at the microscale yield a system of partial differential equations for the characteristic functions which are solved using the finite element method. The effective properties of the polycrystalline material are obtained from the single-crystal thermoelastic properties, crystallographic orientations of the crystallites and the characteristic functions. The proposed methodology is demonstrated by considering electron backscatter diffraction maps of zinc, stainless steel, and natural quartzite rock. Results are presented for homogenized properties such as elastic stiffnesses, thermal expansion coefficients, and seismic wavespeeds, as well as for microscale stress distributions resulting from different macroscale loading conditions. The bulk thermoelastic properties are compared with those obtained using the Voigt, Reuss, Voigt–Reuss–Hill and self-consistent methods. Details are provided regarding a freely available software package that has been developed for the thermomechanical analysis of polycrystalline materials based on the proposed numerical framework.

Keywords: Homogenization; Heterogeneous materials; Bulk properties; Microtexture; Polycrystalline microstructure; Electron backscatter diffraction

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1. Introduction

A large class of technologically important materials, including metals and ceramics, as well as natural materials, such as rocks and ice, are polycrystalline. As such, there is a need for numerical tools that can be used to perform detailed microstructural analysis of polycrystalline materials. Several methods currently exist for the calculation of effective thermoelastic properties of polycrystalline materials given the single-crystal properties and crystallographic orientations of the grains. Previous work on the analysis of polycrystalline materials can be broadly classified into three categories, namely theoretical averaging methods, mean field theories and full-field methods. Examples of theoretical averaging methods include the Voigt [1] and the Reuss [2] methods which are based on the iso-strain and iso-stress assumptions, respectively. It has been shown that the Voigt and the Reuss methods provide upper and lower bounds, respectively, for the bulk elastic stiffnesses [3]. Various theoretical averaging schemes that lie between the two bounds have been proposed, including the Voigt–Reuss–Hill (VRH) arithmetic average [3,4] and the geometric mean [5]. Although these averages closely approximate laboratory-determined bulk elastic properties in some instances, they lack physical justification since they do not account for grain shapes, grain distributions or grain-to-grain interactions. Mean-field theories, such as the self-consistent method [6–9], were developed in an effort to better approximate the response of polycrystalline materials. In the self-consistent method, the average stresses within the grains are obtained by modeling each grain as a separate ellipsoidal inclusion that is embedded within a homogeneous equivalent medium with physical properties that correspond to that of the bulk polycrystalline material. Full-field methods have been developed for the simulation of microscale stress distributions since grain-scale stress concentrations can cause damage or crack initiation. In this context, the finite element (FE) method has been used for the stress analysis of computer-generated polycrystalline microstructures, such as 3D Voronoi polycrystals [10–13]. Numerical simulations of the brittle fracture of polycrystalline materials have been performed using advanced FE techniques and Voronoi microstructures [14,15]. Lebensohn [16] has developed a formulation based on the fast Fourier transform for the viscoplastic analysis of 3D polycrystals. Bishop et al. [17] have performed direct numerical simulations wherein polycrystalline microstructures were embedded throughout a macroscale structure.

Most polycrystalline materials exhibit a pattern of preferred orientations of the crystals, commonly referred to as texture or fabric. In the case of engineered materials, texture is the result of processing history whereas the texture of rocks is due to their natural evolution. It is well known that the texture of polycrystalline materials has a significant influence on bulk properties such as elastic modulus, thermal expansion coefficient, yield strength and fracture toughness. Currently available mainstream methods for collecting crystallographic orientation data can be classified into two distinct categories, namely macrotexture and microtexture techniques. Macrotexture techniques, such as X-ray goniometry and neutron diffraction, enable the determination of bulk texture [18]. They can provide useful information regarding the average orientation data for a large volume of a polycrystalline material. A disadvantage of macrotexture methods is that they cannot capture the detailed spatial variation of crystallographic orientation within a polycrystalline sample. Microtexture techniques, such as electron backscatter diffraction (EBSD), allow for the measurement of the local orientations of the individual crystals within a polycrystalline sample. In recent years, EBSD has become the most popular technique for the measurement of local crystal orientations due to the availability of automated systems which can index patterns at sub-micron spatial resolutions [19,20]. It is now possible to generate detailed microstructural orientation and phase maps using EBSD and to identify individual grains using advanced post-acquisition data analysis software. Subsequently, the bulk properties of the polycrystalline sample can be calculated from the EBSD phase and orientation data using one of the available homogenization schemes. The Voigt, Reuss and VRH are the most widely used methods for the calculation of bulk properties from texture data due to their inherent simplicity and ease of implementation [4,21]. These averaging methods take into account the crystallographic orientations and phase modal fractions but they disregard the shapes and arrangement of the grains, two factors which have been shown to influence the bulk properties of polycrystalline materials [22,23]. Furthermore, these averaging methods are incapable of supplying information in regard to microscale stress and strain distributions induced by macroscale loads.

Numerical methodologies for the analysis of polycrystalline materials have been demonstrated on computer-generated Voronoi-microstructures [10–15]. Much progress has been made in recent years in developing methodologies for the simulation of realistic polycrystalline microstructures [24]. For example, Li et al. [25] have simulated the nano-indentation of polycrystalline aluminum using a Voronoi microstructure with crystallographic orientations imported from EBSD. Dunne et al. [26] reconstructed the grain morphology and crystallographic orientations of a