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A multiscale Taylor model-based constitutive theory describing grain growth in polycrystalline cubic metals

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ABSTRACT

In this work, we have developed a thermodynamically consistent, three-dimensional, finite-deformation-based constitutive theory to describe grain growth due to stress-driven grain boundary motion in polycrystalline cubic metals. The constitutive model has been formulated in a multiscale setting using the Taylor-type homogenization scheme (Taylor, 1938), and it has also been implemented into a computational framework. In our numerical scheme, the mechanical response of a structure at the macroscale level is modeled using the finite-element method whereas at the mesoscale level, the stress-driven grain growth process within a polycrystalline aggregate is handled by phase-field-like simulations.

Using our multiscale constitutive theory and computational framework, we model several boundary value problems involving grain growth in polycrystalline cubic metals. From our coupled finite-element and phase-field simulations, we obtain the following trends: (a) sufficiently stressed polycrystalline metals result in the preferential growth of elastically soft crystal orientations at the expense of elastically hard crystal orientations, and (b) grain growth stagnation effects can be responsible for preventing a polycrystalline aggregate from evolving into a single crystal under stress-driven grain growth conditions. These observations agree well with previously conducted experimental and simulation results available in the literature.

1. Introduction

The ability to control the evolution of crystallographic texture and grain sizes in polycrystalline materials under the action of stimuli e.g. thermal, mechanical, electrical, etc. is a fundamental subject of study in engineering and materials science practice since the overall mechanical and/or electrical properties of a structure/component highly depend on the microstructure it possesses. For polycrystalline bodies, grain boundary motion serves as an important mechanism for microstructure evolution in materials encountered in large-scale structures e.g. rock-forming minerals, polar ice sheets, solar cells, etc. (Ma et al., 2006; Becker et al., 2008) and small-scale microelectronic and nanoelectronic mechanical systems-type devices e.g. interconnects, microelectronic switches, chemical sensors, infrared light detectors, etc. (Gall et al., 2004; Miller et al., 2007a,b).[1]

Since there have been numerous experimentally based works conducted on stress-driven grain boundary motion (grain growth) in polycrystalline metals e.g. see the works of Zielinski et al. (1994, 1995), Winning et al. (2001), Zhang et al. (2001),

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[1] Metals having a face-centered cubic structure such as aluminum, copper, gold and silver are also widely used in the microelectronics industry.

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Sonnweber-Ribic et al. (2006, 2012), Winning (2006), Rupert et al. (2009), etc., we will focus our present discussion on the previously developed constitutive models and numerical capabilities used to study polycrystalline grain growth.

In terms of continuum-based theoretical and computational work, we concentrate on the previous literature regarding elastic-deformation-driven grain growth. With regards to theoretical and numerical efforts, Thompson and co-workers (Frost et al., 1990, 1992; Carel et al., 1994, 1996) model grain growth and texture evolution in polycrystalline metals using a two-dimensional front tracking method. A numerical technique based on the double-grid method was developed by Chen et al. (2004) to study stressed grain growth in polycrystalline metals, but their works were also limited to two-dimensional settings. The constitutive modeling efforts of Tonks et al. (2010); Tonks and Millett (2011), Bhattacharyya et al. (2011) and Kim et al. (2011, 2012) utilize the phase-field method to study the grain growth and microstructure evolution in polycrystalline metals. The phase-field method which is based on a diffuse-interface description of a grain boundary provides a great platform to study realistic i.e. three-dimensional grain growth and texture evolution due to the relative straightforwardness in its numerical implementation.

However, it is important to note that the aforementioned theoretical and numerical works have concentrated on the modeling the polycrystalline grain growth process at the mesoscale level i.e. the response of the macroscale structure as a result of microstructure evolution at the mesoscale level has not been modeled. Since the mechanical properties of a material at the macroscale (engineering component) level depend very strongly on the underlying mesoscale structure i.e. crystallographic texture, grain size etc., we require a multiscale approach to link the mechanical responses at the mesoscale and macroscale levels. To describe the advantages of a multiscale-based approach, consider a macroscale structure which has a polycrystalline microstructure at the mesoscale level. Under the application of thermo-mechanical loads, a deformation field within the macroscale structure will be generated. The mesoscale counterpart of the macroscale deformation field will cause grain growth to take place and the microstructure at the mesoscale level will evolve accordingly. The change of microstructure at the mesoscale level as a result of grain growth will alter the stiffness of the structure at the macroscale level. A change in stiffness of the macroscale structure will in turn alter the macroscale deformation field, and this process will repeat itself until no further microstructure evolution takes place. Hence, the accurate modeling of the grain growth process at the mesoscale level due to the application of thermo-mechanical loads at the macroscale level requires the development of a multiscale-based constitutive model and numerical framework.

To the best of our knowledge, the only effort to study polycrystalline grain growth using a multiscale theoretical and computational framework was that of Chen and Mehraeen (2004). Using their previously developed double-grid method cf. Chen et al. (2004), they have studied stressed grain growth in a two-dimensional setting. However, it is important to note that all the constitutive models mentioned above were not derived in a thermodynamically rigorous manner, and furthermore they also utilize small-strain-based kinematics. The advantage of finite-deformation-based constitutive models is that they will be able to accurately model the grain growth in structures which exhibit large deflections during their deployment cf. the cantilever bending experiments of Gall et al. (2004) and Miller et al. (2007a,b) among others. Furthermore, as shown by the molecular dynamics simulations of Zhang et al. (2004), non-linear elastic strains can have an important effect on the determination of grain growth driving forces.

Therefore, we set out to accomplish the following objectives in this paper: (a) to develop a thermodynamically consistent, multiscale, three-dimensional and finite-deformation-based constitutive model describing grain growth[2] in polycrystalline metals; (b) to numerically implement the multiscale constitutive model in a coupled finite-element and phase-field framework; and (c) to showcase the newly developed constitutive model and computational framework by modeling selected boundary value problems through numerical simulations.

In Section 2, we derive our multiscale constitutive theory based on fundamental balance laws and thermodynamic principles. The developed constitutive model has been implemented into the Abaqus/Standard (2012) finite-element program through a user-material subroutine (UMAT) interface. A separate subroutine which performs the phase-field simulations for the polycrystalline microstructure evolution is also written and embedded into the UMAT subroutine. Algorithmic details of the time integration procedure used to implement the constitutive model are also given in Section 2. In Section 3, we put forth a methodology to determine the material parameters related to grain boundary motion based on the previous works in the literature. Several boundary value problems involving stimulus-driven grain boundary motion in polycrystalline metals are also studied in Section 3 using the developed finite-element and phase-field numerical capability. In Section 4, we attempt to explain some of the trends obtained from the simulation results presented in Section 3 through analytical means. Finally, we conclude and provide directions for future work in Section 5.

2. Multiscale constitutive theory and its computational implementation

2.1. General preliminaries for the multiscale constitutive framework

Consider a homogenized macroscopic continuum body with a characteristic length l_{macro} as shown in Fig. 1a. From a multiscale modeling point of view, the macroscopic continuum body shown in Fig. 1a represents the structure at the *macroscopic/macroscale* level. Let $\overline{\mathcal{R}}$ denote a subregion of the macroscopic continuum body in the *reference* configuration

[2] In the present work, we have neglected the phenomenon of grain coalescence.