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A unified framework for polycrystal plasticity with grain boundary evolution

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Abstract

Plastic deformation in polycrystals is governed by the interplay between intra-granular slip and grain boundary-mediated plasticity. However, while the role played by bulk dislocations is relatively well-understood, the contribution of grain boundaries (GBs) has only recently begun to be studied. GB plasticity is known to play a key role along with bulk plasticity under a wide range of conditions, such as dynamic recovery, superplasticity, severe plastic deformation, etc., and developing models capable of simultaneously capturing GB and bulk plasticity has become a topic of high relevance. In this paper we develop a thermodynamically-consistent polycrystal plasticity model capable of simulating a variety of grain boundary-mediated plastic processes in conjunction with bulk dislocation slip. The model starts from the description of a single crystal and creates lattice strain-free polycrystalline configurations by using a specially-designed multiplicative decomposition developed by the authors. This leads to the introduction of a particular class of geometrically necessary dislocations (GND) that define fundamental GB features such as misorientation and inclination. The evolution of the system is based on an energy functional that uses a non-standard function of the GND tensor to account for the grain boundary energy, as well as for the standard elastic energy. Our implementation builds on smooth descriptions of GBs inspired on diffuse-interface models of grain evolution for numerical convenience. We demonstrate the generality and potential of the methodology by simulating a wide variety of phenomena such as shear-induced GB sliding, coupled GB motion, curvature-induced grain rotation and shrinkage, and polygonization via dislocation sub-grain formation.

Keywords: A. grain boundary plasticity, microstructures, B. crystal plasticity, constitutive behavior, polycrystalline materials

1. Introduction

Engineering materials, particularly metallic alloys, almost always involve polycrystals, characterized by a conglomerate of grains with different crystal orientations[1] separated by grain boundaries (GBs). Deformation models of polycrystalline materials must then necessarily account for grain boundary plasticity, such as that produced by shear-induced grain boundary motion, grain rotation and shrinkage, in addition to bulk or intra-grain plasticity. In fact, both classes of mechanisms often co-occur, such that it is typically quite difficult to distinguish between these in the general context of deformation. Never is this more true than in the well-known cases of recovery, grain growth, and recrystallization [1, 2], which are commonplace processes taking place during high-stress deformation of metallic alloys –particularly at elevated temperature–, and where grain boundaries undergo microstructural transformations contemporaneously with bulk dislocations [3, 4]. Traditionally, however, both types of transformations have been modeled separately, as independent processes that are then linked via some phenomenological coupling (some of these will be discussed below). This has proven unsatisfactory to capture the full complexity observed during microstructural evolution at high stress and/or temperature. It thus urges to take a fresh look at the current theories to explore new avenues to model polycrystal plasticity with co-occurring grain boundary evolution.

The advent of highly-accurate and efficient atomistic methods has enabled the direct simulation of the mechanisms behind grain boundary evolution. Recent applications of molecular dynamics (MD) simulations has opened a new

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[1]With respect to a global *laboratory frame of reference*.