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Deformation patterning in finite-strain crystal plasticity by spectral homogenization with application to magnesium

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Abstract

Complex microstructural patterns arise as energy-minimizers in systems having non-convex energy landscapes such as those associated with phase transformations, deformation twinning, or finite-strain crystal plasticity. The prediction of such patterns at the microscale along with the resulting, effective material response at the macroscale is key to understanding a wide range of mechanical phenomena and has classically been dealt with by simplifying energy relaxation theory or by expensive finite element calculations. Here, we discuss a stabilized Fourier spectral technique for the homogenized response at the level of a representative volume element (RVE). We show that the FFT-based method admits sufficiently high resolution suitable to predict the emergence of energy-minimizing microstructures and the resulting effective response by computing the approximated quasiconvex energy hull. We test the method in the classical single-slip problem in single- and bicrystals. Especially the latter goes beyond the scope of traditional finite element and analytical relaxation treatments and hints at mechanisms of pattern formation in polycrystals. We also demonstrate that the chosen spectral finite-difference approximation, important for removing ringing artifacts in the presence of high contrasts, adds a natural regularization to the non-convex minimization. Finally, the technique is applied to polycrystalline pure magnesium, where we account for the competition between dislocation-mediated plasticity and deformation twinning. These inelastic deformation mechanisms result in complex texture evolution paths at the polycrystalline mesoscale and are simulated within RVEs of varying grain size and texture by a constitutive crystal plasticity model with an effective, volume fraction-based description of twinning.

Keywords: Homogenization, Spectral Methods, Polycrystal, Microstructure, Magnesium

1. Introduction

Magnesium (Mg) and magnesium alloys of various compositions have drawn interest for structural applications, primarily due to their high specific strength and low density (Pollock, 2010; Dixit et al., 2015). However, predicting the macroscopic mechanical response of bulk polycrystalline magnesium while also resolving the local fields, particularly interactions of twins with grain boundaries, presents an open challenge. The hexagonal closed-packed (hcp) crystal structure of Mg results in anisotropic inelastic deformation mechanisms (Graff et al., 2007; Stanford et al., 2011), remarkably low ductility and an asymmetric tension-compression behavior (Máthis et al., 2011; Park et al., 2014; Zachariah et al., 2013; Kurukuri et al., 2014). Dislocation slip and deformation twinning occur as competing mechanisms, and their mechanistic influences drive complex microstructure evolution paths observed in magnesium polycrystals (Agnew and Duygulu, 2005; Chang et al., 2017). It is hence important to understand and to enable the prediction of mesoscale microstructure evolution by high-fidelity methods to gain insight into the link between processing conditions, resulting microstructure and, ultimately, effective material properties. Simulations, in principle, must span a wide range of length and time scales to accurately capture interactions between twinning and dislocation slip, both of which are affected by the polycrystalline texture and grain size distribution. To this end, a combination of

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