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Stochastic modeling of discontinuous dynamic recrystallization at finite strains in hcp metals

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Abstract

We present a model that aims to describe the effective, macroscale material response as well as the underlying mesoscale processes during discontinuous dynamic recrystallization under severe plastic deformation. Broadly, the model brings together two well-established but distinct approaches – first, a continuum crystal plasticity and twinning approach to describe complex deformation in the various grains, and second, a discrete Monte-Carlo-Potts approach to describe grain boundary migration and nucleation. The model is implemented within a finite-strain Fast Fourier Transform-based framework that allows for efficient simulations of recrystallization at high spatial resolution, while the grid-based Fourier treatment lends itself naturally to the Monte-Carlo approach. The model is applied to pure magnesium as a representative hexagonal closed packed metal, but is sufficiently general to admit extension to other material systems. Results demonstrate the evolution of the grain architecture in representative volume elements and the associated stress–strain history during the severe simple shear deformation typical of equal channel angular extrusion. We confirm that the recrystallization kinetics converge with increasing grid resolution and that the resulting model captures the experimentally observed transition from single- to multi-peak stress–strain behavior as a function of temperature and rate.

Keywords: Recrystallization, Monte-Carlo, Homogenization, Magnesium, Polycrystal

1. Introduction

Strengthening metals through grain refinement based on the relation of Hall (1951) and Petch (1953) can be achieved by a number of forming processes that induce a microstructural reorganization of the polycrystalline grain structure, with processes ranging from asymmetric roll bonding and asymmetric rolling to high-pressure torsion and equal channel angular extrusion (ECAE) (see e.g. Hallberg (2011); Sakai et al. (2014)). Controlling a material's performance through such processing routes calls for accurate structure–property relations as well as for efficient computational models that predict the underlying microstructural mechanisms as a function of the thermo-mechanical process parameters. Here, we present a micromechanical model which describes recrystallization, one of the key underlying causal mechanisms of changes to the grain structure in metals, encountered e.g. during the ECAE process.

Recrystallization occurs in various ways. *Static recrystallization* is a temperature-driven process that occurs under slowly-varying, creep-like loading conditions such as during annealing (Sakai et al., 2014; Zhang et al., 2013), where the average grain size increases with a negative impact on the strength properties. This can be overcome, e.g., through alloying by rare earth metals, as shown for Mg-Zn-Zr alloys enriched with Er and undergoing static recrystallization at high temperatures (Zhang et al., 2013). Occurring at higher loading rates, *dynamic recrystallization*¹ emerges from the competition between recrystallization and continued plastic deformation such as during ECAE. It is further

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¹Note that *dynamic* refers to the fact that the recrystallization mechanisms occur during continued plastic deformation. It does not refer to inertia or shocks.

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