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M. Jafari, M. Jamshidian, S. Ziaei-Rad, D. Raabe, F. Roters

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Constitutive modeling of strain induced grain boundary migration via coupling crystal plasticity and phase-field methods

M Jafari[a], M Jamshidian[a,*], S Ziaei-Rad[a], D Raabe[b], F Roters[b]

[a] *Department of Mechanical Engineering, Isfahan University of Technology, Isfahan 84156-83111, Iran*
[b] *Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany*

Abstract

We have developed a thermodynamically–consistent finite-deformation-based constitutive theory to describe strain induced grain boundary migration due to the heterogeneity of stored deformation energy in a plastically deformed polycrystalline cubic metal. Considering a representative volume element, a mesoscale continuum theory is developed based on the coupling between dislocation density-based crystal plasticity and phase field methods. Using the Taylor model-based homogenization method, a multiscale coupled finite-element and phase-field staggered time integration procedure is developed and implemented into the Abaqus/Standard finite element package via a user-defined material subroutine. The developed constitutive model is then used to perform numerical simulations of strain induced grain boundary migration in polycrystalline tantalum. The simulation results are shown to qualitatively and quantitatively agree with experimental results.

Keywords: Constitutive modeling, Strain induced boundary migration, Crystal plasticity, Phase field, Finite elements

1. Introduction

Polycrystalline microstructure of metallic materials can be tailored to specific engineering needs by optimizing the evolution of microstructure via grain boundary migration (Stojakovic et al., 2008; Ciulik and Taleff, 2009). Therefore, understanding the mechanisms and driving forces for grain boundary migration is necessary for producing metals with superior properties via controlling the microstructural characteristics such as crystallographic texture and grain size. During plastic deformation, most of the plastic work is converted into heat. However, a small portion of the plastic work is stored in dislocation structures, the so-called *stored deformation energy* (Anand et al., 2015). Plastic anisotropy of grains in a polycrystalline microstructure results in a stored energy difference across grain boundaries which in turn can provide a driving force sufficient for grain boundary migration in a number of processes (Humphreys and Hatherly, 2004; Raabe, 2014). Strain induced grain boundary migration (SIBM) is known as the migration of a pre-existing grain boundary segment driven by the stored energy difference across that grain boundary (Humphreys and Hatherly, 2004; Raabe, 2014). While keeping its original crystallographic orientation, the region swept by a grain

*Corresponding author. Email: jamshidian@cc.iut.ac.ir