International Journal of Plasticity 80 (2016) 38–55

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

An integrated full-field model of concurrent plastic deformation and microstructure evolution: Application to 3D simulation of dynamic recrystallization in polycrystalline copper

Pengyang Zhao [a], Thaddeus Song En Low [a], Yunzhi Wang [a,*], Stephen R. Niezgoda [a,b,*]

[a] *Department of Materials Science and Engineering, The Ohio State University, United States*
[b] *Department of Mechanical and Aerospace Engineering, The Ohio State University, United States*

ARTICLE INFO

Article history:
Received 16 September 2015
Received in revised form 30 November 2015
Available online 5 January 2016

Keywords:
A. Dislocations
A. Microstructures
A. Thermomechanical processes
B. Crystal plasticity
B. Polycrystalline material

ABSTRACT

Many time-dependent deformation processes at elevated temperatures produce significant concurrent microstructure changes that can alter the mechanical properties in a profound manner. Such microstructure evolution is usually absent in mesoscale deformation models and simulations. Here we present an integrated full-field modeling scheme that couples the mechanical response with the underlying microstructure evolution. As a first demonstration, we integrate a fast Fourier transform-based elasto-viscoplastic (FFT-EVP) model with a phase-field (PF) recrystallization model, and carry out three-dimensional simulations of dynamic recrystallization (DRX) in polycrystalline copper. A physics-based coupling between FFT-EVP and PF is achieved by (1) adopting a dislocation-based constitutive model in FFT-EVP, which allows the predicted dislocation density distribution to be converted to a stored energy distribution and passed to PF, and (2) implementing a stochastic nucleation model for DRX. Calibrated with the experimental DRX stress–strain curves, the integrated model is able to deliver full-field mechanical and microstructural information, from which quantitative description and analysis of DRX can be achieved. It is suggested that the initiation of DRX occurs significantly earlier than previous predictions, due to heterogeneous deformation. DRX grains are revealed to form at both grain boundaries and junctions (e.g., quadruple junctions) and tend to grow in a wedge-like fashion to maintain a triple line (not necessarily in equilibrium) with old grains. The resulting stress redistribution due to strain compatibility is found to have a profound influence on the subsequent dislocation evolution and softening.

1. Introduction

Many thermomechanical processes and high temperature applications of materials involve a coupled evolution of micromechanical fields, local defect populations, and microstructural constituents including precipitates and grains. For

* Corresponding authors. Department of Materials Science and Engineering, The Ohio State University, United States.
E-mail addresses: wang.363@osu.edu (Y. Wang), niezgoda.6@osu.edu (S.R. Niezgoda).

http://dx.doi.org/10.1016/j.ijplas.2015.12.010
0749-6419/

instance, during hot deformation crystalline materials with low stacking fault energy (SFE) often undergo dynamic recrystallization (DRX) wherein new grains will continue to nucleate and grow (Sakai and Jonas, 1984; Sakai et al., 2014), altering the population, mutual elastic interaction, and subsequent motion of dislocations in a distinctive manner. These microstructural changes are difficult to capture through purely mechanical laws (Roters et al., 2010). The continued adoption of new computational strategies for accelerated development of materials, such as Integrated Computational Materials Engineering (Allison et al., 2006; Allison, 2011), for materials processed through thermomechanical routes or materials exposed to thermal and mechanical extremes in-service requires modeling and simulation tools that integrate both the mechanical and microstructural aspects in a fully coupled manner.

Within the broader solid mechanics and materials science communities, mature computational approaches exist to study, separately, the deformation of heterogenous materials and microstructure evolution. On one hand, the field of crystal plasticity has benefited substantially from multi-scale experiments and simulations linking mechanical properties of materials with the evolution of contained structural defects such as dislocations under an applied stress or displacement field. At the mesoscale, this understanding has been implemented into physics-based constitutive theories (Arsenlis and Parks, 2002; Arsenlis et al., 2004; Cheong and Busso, 2004; Ma et al., 2006; Gao and Huang, 2003; Beyerlein and Tomé, 2008) and implemented into homogenized deformation models such as self-consistent schemes (Lebensohn and Tomé, 1993; Niezgoda et al., 2014) or full-field simulations such as finite element based crystal plasticity (FE-CP) (Kalidindi et al., 1992; Beaudoin et al., 1995; Roters et al., 2010) or fast Fourier transform (FFT) based crystal plasticity (FFT-CP) models (Lebensohn, 2001; Lebensohn et al., 2012; Eisenlohr et al., 2013). On the other hand, the microstructural evolution in crystals, such as grain growth (Chen and Yang, 1994; Kazaryan et al., 2002; Moelans et al., 2008b), static recrystallization (Moelans et al., 2013), rafting in superalloy (Zhou et al., 2010; Gaubert et al., 2010) and many other phenomena (Chen, 2002; Wang and Li, 2010) have been well studied using phase-field (PF) simulations. The non-boundary tracking field description of microstructures and the incorporation of thermodynamics-based free energy formulation have made PF a very powerful and robust tool in simulating and predicting the microstructural evolution often in a quantitative manner (Chen, 2002; Boettinger et al., 2002; Shen et al., 2004; Moelans et al., 2008b; Steinbach, 2009; Wang and Li, 2010).

In recent years, efforts have been made towards developing CP models that can incorporate microstructure features to study plastic deformation of materials such as austenitic steels, TRIP steels, brass, TWIP steels and shape memory alloys that deform not only by dislocation slips but also by displacive phase transformation mechanisms. For instance, frameworks (Thamburaja and Anand, 2001; Turteltaub and Suiker, 2005; Lan et al., 2005; Manchiraju and Anderson, 2010) have been developed to incorporate martensitic transformations into the flow rules. Mechanical twinning, which is of great importance to the plasticity of many BCC metals as well as FCC metals with low SFE, has also been incorporated into FE-CP models (Kalidindi, 1998; Staroselsky and Anand, 1998; Salem et al., 2005; Steinmetz et al., 2013; Zhang et al., 2008). Atomistically-informed dislocation-based models have also been developed recently and applied to single crystal (Cereceda et al., 2016). In addition, microstructure modeling techniques such as cellular automata and phase-field have also been applied to the study of mechanics-induced microstructural evolution such as static recrystallization (Hesselbarth and Göbel, 1991; Raabe, 2002; Takaki et al., 2007; Moelans et al., 2013; Chen et al., 2015). These models, while providing certain connection between microstructure and crystal plasticity, still lack a dynamic coupling between the two. On the other hand, phase-field models incorporating either continuum plasticity (Gaubert et al., 2010) or dislocation density fields (Zhou et al., 2010) have also been developed to study rafting in Ni-based superalloys. These models are mainly rooted in the PF framework and significant advances are required in order to generalize the approach and incorporate a wider range of existing constitutive theories.

Regarding the simulation of DRX, there have been models aiming to couple deformation with microstructure evolution. In the models of Ding and Guo (2001) and Takaki et al. (2008), the growth of DRX grains was modeled by cellular automaton and PF, respectively, and the phenomenological Kocks-Mecking model (Mecking and Kocks, 1981) was used to model the evolution of average dislocation density, which in return influenced the mechanics through its square root relationship with the flow stress. Recently Takaki et al. (2014) extended their previous work by replacing the flow stress model with an elastic–plastic FE, intending to establish a full coupling model. However, the mechanical behavior was still considered in a macroscopic level in the sense that an average dislocation density was assumed for each grain which evolved according to the Kocks-Mecking model (Mecking and Kocks, 1981). DRX, on the other hand, occurs at a sub-grain level where grain boundary (GB) bulging (Ponge and Gottstein, 1998; Wusatowska-Sarnek et al., 2002; Miura et al., 2007) or other possible mechanisms (Rollett et al., 2004) might operate to initiate the nucleation of new grains. This length scale separation implies that a "homogenized" coupling scheme (Takaki et al., 2014) may limit its application in exploring the underlying physics. Another recent DRX model by Popova et al. (2015), which couples FE-CP with a probabilistic cellular automata, successfully captured both texture and mechanical feature during the DRX in magnesium. However, only geometrically necessary dislocations (GND) were considered with the effect of statistically stored dislocations (SSD) being ignored, and the two-dimensional (2D) simulation ignores important microstructural features (e.g., the triple/quadruple grain junctions (Miura et al., 2005)) when analyzing the dynamics of DRX grains.

In this paper, we present an integrated modeling scheme of fully coupling the mechanical response with the underlying microstructure evolution by employing FFT-CP and PF. This novel scheme is then implemented in simulating dynamic recrystallization in polycrystalline copper in three-dimensions (3D). Quantitative agreement between simulations and