Journal of the Mechanics and Physics of Solids 68 (2014) 107–133

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

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

Mechanism-based crystal plasticity modeling of twin boundary migration in nanotwinned face-centered-cubic metals

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ARTICLE INFO

Article history:
Received 4 March 2013
Received in revised form
23 September 2013
Accepted 14 March 2014
Available online 3 April 2014

Keywords:
Nanotwinned metals
Interface effects
Crystal plasticity
Twin boundary migration
Finite element analysis

ABSTRACT

Nanotwinned (nt) metals are an important subset of nanostructured materials because they exhibit impressive strength and ductility. Several recent investigations on nt face-centered-cubic (FCC) metals indicate that their macroscopic responses emerge from complex microscopic mechanisms that are dominated by dislocation–TB interactions. Under applied stimulus, nt microstructures evolve through migration of twin boundaries (TBs) that may have implications on the material strength and stability. This work focuses on modeling TB migration within finite element framework in an explicit manner and studying its effects on the micromechanics of twinned FCC metals under quasi-static loading conditions. The theoretical setting is developed using three-dimensional single crystal plasticity as a basis wherein the plastic slip on the $\{111\}\langle\bar{1}10\rangle$ slip systems in an FCC crystal structure is modeled as visco-plastic behavior. Owing to their governing role, twins are modeled as discrete lamellas with full crystallographic anisotropy. To model TB migration, an additional visco-plastic slip-law for twinning partial systems ($\{111\}\langle11\bar{2}\rangle$) based on the nucleation and motion of twin partial dislocations is introduced. This size-dependent constitutive law is presumed to prevail in the vicinity of the TB and naturally facilitates TB migration when combined with a twinning condition that is based on the accrual of the necessary shear strain. The constitutive development is implemented within a finite element framework through a User Material (UMAT) facility within ABAQUS/STANDARD®. Detailed micromechanics simulations on model microstructures involving single-grained and polycrystalline topologies are presented.

1. Background

Interfaces are ubiquitous features in crystalline and non-crystalline material microstructures. In crystalline materials they may prevail as boundaries between crystallographic misorientations, inclusions embedded in grains, and several others. Indeed, they are an integral part of microstructural engineering geared toward strengthening and toughening of crystalline metals. With recent advancements in microstructural engineering, nanostructured materials have gained tremendous prominence whereby the characteristic spacing between such interfaces that act as barriers to dislocation motion can be controlled well below the micrometer regime, resulting in substantially enhanced yield strength, sometimes by an order of magnitude over their conventional coarse-grained counterparts. Among the variety of strategies that have been devised,

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http://dx.doi.org/10.1016/j.jmps.2014.03.006
0022-5096/

nanotwinned (nt) microstructures have triggered significant interest primarily arising from the exciting experimental results reported by Lu et al. (2004) and Lu et al. (2009) on polycrystalline nt-Cu that exhibit simultaneous enhancement/retaining of the yield strength and ductility with decreasing TB spacing λ. Some of the broad characteristics may be summarized as follows:

1. Enhancement of the yield strength σ_y with decreasing twin thickness λ that follows a Hall–Petch behavior (i.e. $\sigma_y \sim 1/\sqrt{\lambda}$).
2. Decrease in σ_y below a critical λ (yield softening).
3. Enhanced strain hardening, rate-sensitivity and ductility with decreasing λ.
4. Microstructural evolution via TB migration.

Several analytical and computational investigations have been performed on nt face-centered-cubic (FCC) materials to understand the deformation mechanisms in twinnable materials, mainly Cu (Asaro and Suresh, 2005; Dao et al., 2006; Wang et al., 2007; Shan et al., 2008; Chen et al., 2008; Hu et al., 2009; Kulkarni and Asaro, 2009; Wu et al., 2009; Shabib and Miller, 2009; Li and Ghoniem, 2009; Anderoglu et al., 2010; Brown and Ghoniem, 2009, 2010; Zhu and Li, 2010; Wang et al., 2010b; Zhou et al., 2010; Li et al., 2011; Jang et al., 2012), but also in gold (Seo et al., 2011), palladium (Stukowski et al., 2010; Idrissi et al., 2011), silver (Bufford et al., 2011) and aluminum (Zhu et al., 2004; Daphalapurkar and Ramesh, 2012). While the first three aspects have been modeled using continuum approaches (Dao et al., 2006, 2007; Zhu et al., 2007; Jérusalem et al., 2008; Zhou et al., 2010; Li et al., 2010; Mirkhani and Joshi, 2011) the mechanics modeling of TB migration in nt-microstructures has not been dealt within a continuum micromechanics framework. Yet, it is important to model the mechanics of such twinned microstructures to enable designing applications that perform optimally (Hsiao et al., 2012). For example, TB spacing has been shown to influence electromigration-induced void generation in Cu, which is critical in electronics applications (Chen et al., 2008).

This work presents micromechanics modeling of the size-dependent TB migration and investigating its effects on the quasi-static macroscopic behavior of model nt microstructures within crystal plasticity framework. Most of the existing crystal plasticity models for nt metals ignore the discreteness of twins within a crystal by homogenizing their effect via rule-of-mixtures law for the stress and strain partitioning. Further, the effect of TBs on strength enhancement is modeled by writing plastically anisotropic slip laws for slip systems parallel and non-coplanar to the TBs. Compared to this *homogenized* twin crystal plasticity modeling, the present work is based on the viewpoint that it is important to retain the discreteness of twinned structure within individual crystals, referred to as Discrete Twin Crystal Plasticity (DTCP) (Mirkhani and Joshi, 2011). Although the microstructural length-scales in the homogenized and DTCP models are in the same range, retaining the discreteness of twin lamellas enables explicit modeling of TB migration and investigating the micromechanical effects that may not be realizable if the twin motif is homogenized. The salient features of the present work are

a. Development of a mechanism-based constitutive framework based on twin partial (TP) slip activity to model TB migration. The model naturally predicts the direction and speed of TB migration as a function of underlying TP activity.
b. Computational implementation of this model as a User Material subroutine (UMAT) based on the rate-dependent FCC single crystal plasticity of Asaro (1983) within ABAQUS/STANDARD®.
c. Micromechanics investigation of TB migration for single and multiple TBs within a crystal.
d. Micromechanics investigation of TB migration in a polycrystalline setting.

The focus of this work is on modeling the evolution of microstructures with pre-existing twins (e.g. growth twins), but the approach can readily be extended to modeling the formation of twin nuclei and their evolution under mechanical loading as well.

2. A brief review of TB migration in FCC metals

Before presenting the DTCP model and the results of TB migration simulations, we briefly review some of the key results from the experimental and modeling literature on TB migration in nt-FCC metals that are important for the purpose of present modeling approach. For a detailed account of twinning the reader is referred to the seminal review by Christian and Mahajan (1995). More recently, Niewczas (2007) and Zhu et al. (2012) have compiled excellent reviews on twinning in FCC crystals and in nanocrystalline materials, respectively.

2.1. Experimental observations

Early experimental observations on the mechanisms associated in twinned polycrystalline Cu indicate that TBs can be significant sources of dislocations, especially in the initial plastic flow regime (Flinn et al., 2001; Field et al., 2004). Experiments by Konopka et al. (2000) on Cu and austenitic steel showed that TBs may act as efficient dislocation sources, providing a basis for the correlation between the reduction in the flow stresses with increasing TB density. *In-situ* TEM experiments on nt-Cu reveal systematic activation of Shockley twin partial dislocation (TPs) from TB–GB triple junction