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Quantifying the influence of twin boundaries on the deformation of nanocrystalline copper using atomistic simulations

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ABSTRACT

Over the past decade, numerous efforts have sought to understand the influence of twin boundaries on the behavior of polycrystalline materials. Early results suggested that twin boundaries within nanocrystalline face-centered cubic metals have a considerable effect on material behavior by altering the activated deformation mechanisms. In this work, we employ molecular dynamics simulations to elucidate the role of twin boundaries on the deformation of ⟨100⟩ columnar nanocrystalline copper at room temperature under uniaxial strain. We leverage non-local kinematic metrics, formulated from continuum mechanics theory, to compute atomically-resolved rotational and strain fields during plastic deformation. These results are then utilized to compute the distribution of various nanoscale mechanisms during straining, and quantitatively resolve their contribution to the total strain accommodation within the microstructure, highlighting the fundamental role of twin boundaries. Our results show that nanoscale twins influence nanocrystalline copper by altering the cooperation of fundamental deformation mechanisms and their contributed role in strain accommodation, and we present new methods for extracting useful information from atomistic simulations. The simulation results suggest a tension–compression asymmetry in the distribution of deformation mechanisms and strain accommodation by either dislocations or twin boundary mechanisms. In highly twinned microstructures, twin boundary migration can become a significant deformation mode, in comparison to lattice dislocation plasticity in non-twinned columnar microstructures, especially during compression.

1. Introduction

Improving the mechanical properties (e.g., strength, ductility, fatigue resistance, etc.) of materials for advanced functionality has motivated recent work to investigate the influence of altering a material's substructure. One common approach for improving strength in metals is to reduce the average grain size, as described by the Hall–Petch relationship (Hall, 1951; Petch, 1953). The Hall–Petch effect (i.e., strengthening with decreasing average grain size) in polycrystalline materials is based on the idea that interfaces between grains (i.e., grain boundaries (GBs)), serve to block the migration of lattice

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dislocations and suppress conventional dislocation strain accommodation. Higher resolved stresses are then required to overcome these obstacles, thereby, increasing the strength of a material. However, early findings showed that as material strength increased due to grain size reduction, there is a simultaneous decrease in material ductility (Gleiter, 1989; Koch, 2003; Ma, 2003). Therefore, recent efforts have focused on simultaneously improving strength and ductility in metallic materials using a variety of approaches (Ertorer et al., 2009; Karimpoor et al., 2003; Ma, 2006; Shen et al., 2008; Valiev et al., 2002; Youssef et al., 2005; Zhao et al., 2008).

As grain size is reduced to create nanocrystalline (NC) materials, the influence of GBs on macroscopic behavior is more substantial and alternative deformation mechanisms begin to operate (Capolungo et al., 2007; Chen et al., 2003; Derlet et al., 2006; Frøseth et al., 2004, 2005; Kumar et al., 2003; Liao et al., 2003; Meyers et al., 2006; Schiotz and Jacobsen, 2003; Schiotz, 2004; Shan et al., 2004; Tschopp and McDowell, 2008; Van Swygenhoven and Derlet, 2001; Van Swygenhoven and Weertman, 2006; Wang et al., 2012; Yamakov et al., 2004; Zhang et al., 2013; Zhu and Lu, 2012). However, as Schiotz and Jacobsen (2003) noted, a transition from dislocation-dominated to GB-mediated plasticity in Cu occurs at an average grain size that exhibits maximum strength in NC systems. These results indicate that there are inherent length-scales (i.e., average grain size and mean dislocation slip distance) that affect deformation and the role of nanoscale interfaces in NC metals is fundamental to material behavior. Nanoscale interfaces, such as coherent twin boundaries (TBs), have been the subject of recent endeavors aimed at improving strength without limiting other physical properties (Karimpoor et al., 2003; Lu et al., 2009; Ma et al., 2004; Wei, 2011; Zhu et al., 2011; Zhao et al., 2006). This is in part motivated by work from Lu et al. (2004) showing that nanoscale growth twins in NC Cu led to significant improvement in strength while preserving electrical conductivity. These findings suggest that coherent TBs within nanoscale grains hinder the migration of lattice dislocations and lead to strain hardening, similar to other GBs, but do not decrease electrical conductivity. Furthermore, recent findings by Wang et al. (2007) have shown that dislocations can preferentially be emitted from the intersection of a GB and TB to induce TB migration in Cu during tensile deformation. This indicates the potential role of nanoscale twins to affect the deformation behavior in NC metals during plasticity by altering the barrier for dislocation nucleation and serving as an obstacle for migrating lattice dislocations. In more recent work by Brons et al. (2013,), TB mechanisms, such as detwinning, were observed to coincide with abnormal grain growth observed in nanoindentation of NC Cu thin films at cryogenic temperatures, especially in ⟨100⟩ textured columnar NC Cu. The evolution of twin density within the various regions of the indented thin film suggests their role in strain accommodation and influence on other nanoscale mechanisms as a function of orientation and resolved stress state.

To further study the role of TBs in face-centered cubic metals, other efforts have utilized molecular dynamics (MD) simulations. Frøseth et al. (2004) used NC Cu and Ni structures to show that the influence of TBs on the deformation mechanisms is not identical for all fcc metals. They explained these differences by analyzing the generalized planar fault (GPF) energy curves for both dislocation nucleation and TB migration. In addition, their simulations show that emitted dislocations prefer to slip on planes of maximum Schmid factor, and TB migration alone is not responsible for strain accommodation in nanotwinned (NT) Cu and Ni. In addition, recent atomistic simulations by Wu et al. (2011) on Cu detail critical dislocation mechanisms as migrating dislocations interact with TBs. Their rational is based on the fact that TB migration must be accompanied by other strain accommodation mechanisms in NT Cu. Therefore, atomistic calculations were employed to elucidate the critical TB spacing for determining the transition of dominant mechanisms that involve dislocation/TB interactions. Their results showed that a maximum in the strength of NT Cu, as a function of TB spacing, coincides with this mechanism transition. At smaller twin spacings, Li et al. (2010) showed that dislocation nucleation controlled behavior was fundamental to a softening trend in NT metals. Their MD simulations suggest that the strength of NT Cu is dependent on both the average grain size and TB spacing. Furthermore, they conclude that in structures with smaller-spaced TBs, dislocations are nucleated at the TB-GB intersection (due to a local high stress concentration) and glide along the TBs inducing TB migration, as observed earlier by Wang et al. (2007). Therefore, TBs can be preferred nucleation pathways for dislocations and possibly act as sites for further plastic deformation.

These experimental and computational results have led to a significant understanding of the influence of TBs in nanotwinned metals, and have provided insight into the vital structure–property relationships that govern material behavior. However, many conclusions of previous MD simulations about the cooperation/competition of different nanoscale deformation mechanisms, as a result of TBs in the microstructure, have been mostly qualitative. There have been more recent efforts, however, aimed at quantifying plastic deformation within nanocrystalline metals using post-processing methods and atomistic simulations, such as Stukowski et al. (2010) and Vo et al. (2008). In Stukowski et al. (2010), the identification and determination of dislocation and planar fault densities is provided in the context of twinning effects in equiaxed NC Cu and Pd. While in Vo et al. (2008), the strain contribution of dislocations and GB sliding was quantified in equiaxed NC Cu during uniaxial compression as a function of strain rate and grain size. These efforts represent a significant stride in (1) understanding the nanoscale strain accommodation mechanisms in nanocrystalline metals and (2) developing innovative tools for data analysis from atomistic simulations. Inspired by these efforts and the initial findings/questions of Brons et al. (2013), our objective is to elucidate the influence of grown-in TBs in ⟨100⟩ textured columnar NC Cu on the active nanoscale deformation mechanisms, especially the interplay of dislocation slip and TB migration, and their role in strain accommodation within the microstructure using large-scale MD simulations and post-processing methods formulated from continuum mechanics theory. To accomplish these objectives, we leverage non-local kinematic metrics and atomistic fields to compute the evolution and interplay of different deformation mechanisms commonly observed within NC fcc metals. In addition, we quantitatively show how TBs and the loading direction influence the role of nanoscale processes in accommodating strain within