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Influence of grain boundary structure and topology on the plastic deformation of nanocrystalline aluminum as studied by atomistic simulations

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ABSTRACT

Nanocrystalline materials, with grain sizes below 100 nm, have been the subject of many research studies in the recent past. At these reduced grain sizes, grain boundaries (GBs) play a very important role in the deformation of such materials. Large scale atomistic simulations that are often used to illuminate the deformation mechanisms in such materials must accurately account for the topology, structure and network of GBs. In this work, we perform atomistic simulations on nanocrystalline aluminum under tensile loading, using a structure with a relaxed GB network obtained from three-dimensional grain growth simulations, and compare the results to that obtained from structures generated using the Voronoi tessellation method. The results show that the grain growth sample results in consistently higher macroscopic stresses when compared to the Voronoi tessellated microstructures. The latter, additionally, tend to overestimate GB deformation, whilst simultaneously underestimating the deformation due to dislocation slip. More importantly, twinning is observed in multiple grains in the grain growth sample, in contrast to the near absence in Voronoi tessellated microstructures. The results are carefully discussed in terms of sample characteristics, stacking fault energies, and GB structure and network.

1. Introduction

Nanocrystalline (NC) materials have evoked increasing interest in recent decades, spurred both by advances in processing techniques and by insights obtained from computational materials science (Gleiter, 1989; Kumar et al., 2003; Wolf et al., 2005; Meyers et al., 2006; Van Swygenhoven and Weertman, 2006). Such materials, with grain sizes below 100 nm, show promise for a wide variety of applications due to enhanced properties, like high strength up to grain sizes of approximately 10 nm which is usually attributed to the Hall-Petch effect (Kumar et al., 2003). Although generally associated with reduced ductility (Van Swygenhoven and Weertman, 2006), recent investigations have suggested that exploiting key mechanisms like stress-assisted grain growth might lead to improved ductility (Valiev et al., 2002; Gianola et al., 2006).

Due to the increased fraction of grain boundaries (in comparison to coarse-grained ($d > 1\ \mu$m) counterparts), the role of grain boundaries (GBs) is significantly enhanced – and sometimes completely different – in nanocrystalline metals (Wolf

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et al., 2005; Meyers et al., 2006). Large scale atomistic simulations have played a crucial role in detailing the role of GBs in NC materials (Farkas, 2013; Hahn and Meyers, 2015). Such simulations have shown that the paucity of intra-granular dislocation sources like the Frank-Read source results in GBs acting as sources and sinks for dislocations, i.e. regions of stress concentration in GBs act as nucleation sites for dislocations, which can then propagate through the grain before being absorbed in another GB (Schiøtz, 2004). Additionally, GB defect structures such as ledges act as temporary pinning points for the nucleated and/or propagating dislocations (Van Swygenhoven et al., 2006). Furthermore, the inverse Hall-Petch (HP) behavior observed in almost all NC metals is due to a transition with decreasing grain size from that dominated by intra-crystalline deformation via dislocation glide to grain boundary sliding (Schiøtz et al., 1998; Schiøtz and Jacobsen, 2003; Van Swygenhoven et al., 1999) triggered by atomic shuffling and/or stress assisted diffusion (Van Swygenhoven and Caro, 1998; Van Swygenhoven and Derlet, 2001).

It clearly follows from the above that GB and related features, i.e. topology, structure – with its constituent defects – together with the complete network can significantly affect the properties of nanocrystalline materials; to an extent this influence is significantly higher than what is known for conventional coarse-grained materials (Hirth, 1972, 1974). Atomistic models must hence account for the right GB topology and network whilst modeling the deformation behavior of nanocrystalline materials. Most such studies, however, make use of the well-known Voronoi tessellation (Voronoi, 1908) technique to produce artificial microstructures (e.g. Derlet and Van Swygenhoven, 2003; Van Swygenhoven et al., 2006; Brandl et al., 2011; Schäfer and Albe, 2012; Tucker et al., 2012; Wu et al., 2013; Junge and Molinari, 2014). Periodic microstructures generated by this method, using random seeds as grain centers, evidence topological and statistical properties that generally deviate largely from those of realistic microstructures (Xu and Li, 2009); for example, the grain size distribution is limited to the Poisson-Voronoi distribution (Gross and Li, 2002) and differs greatly from those found in experiments (Mason et al., 2015). Very few atomistic simulation studies make use of initial structures that are generated by other means and can be deemed to contain more realistic GB topology and network (Li and Xu, 2011; Tucker and Foiles, 2015; Thomas et al., 2016; Panzarino et al., 2016; Gruber et al., 2017). Although certain properties of Voronoi tessellated microstructures can be tailored to reflect those of real microstructures (Zhang et al., 2011; Leonardi et al., 2012, 2013), an important but limiting aspect of Voronoi tessellated microstructures is that GBs are restricted to planar interfaces.

Indeed, usage of simple starting configurations such as Voronoi tessellated microstructures or bi-crystalline setups with planar interfaces has been the norm in atomistic simulations, particularly for studies of dislocation GB interactions (Tucker and McDowell, 2011; Tschopp and McDowell, 2008; Spearot et al., 2007), or even GB fracture (Möller and Bitzek, 2014). However, such simplistic setups can inhibit important mechanisms and features that are observed in experiments, thus blurring our understanding of the deformation behavior. For instance, recent investigations on atom probe tomography informed atomistic samples containing γ/γ' microstructure of a Ni-base superalloy show that important dislocation interactions like collinear reaction and the knitting out of dislocations, together with dislocation core structures and network can be easily suppressed by simplistic setups (Prakash et al., 2015a). There is hence an impetus towards usage of direct experimental microstructures in simulation-based investigations. The availability of versatile atomistic sample generation tools (Prakash et al., 2016a) has now made this a possibility. Nonetheless, procurement of experimental datasets and their usage in simulations remains challenging (Li and Xu, 2011; Prakash and Bitzek, 2017). An alternative method is to use the output of meso-scale models, where the microstructure generated is based on a sound foundation of physical laws, and can be generally considered to be more realistic (Prakash and Bitzek, 2017) than artificially generated samples like the Voronoi structures.

The usage of realistic microstructures in atomistic simulations also has implications for constitutive modeling at the continuum scale. The predictive power of continuum scale models can be improved significantly through the information obtained from atomistic simulations (Cereceda et al., 2016; Amodeo et al., 2016); however, this hinges strongly upon the ability of the model to capture the mechanistic underpinnings (Taupin et al., 2015; Sun et al., 2016) of the deformation. Constitutive models for NC materials, particularly mechanism-based models (e.g. (Asaro and Suresh, 2005; Yuan et al., 2015; Khan and Liu, 2016)), would hence benefit immensely from the details on individual deformation mechanisms that can be obtained from atomistic simulations.

In this work, we study the influence of GB curvature, topology and network on the deformation behavior of synthetic polycrystalline microstructures. To this end, we perform simulations on an atomistic configuration generated from a snapshot produced by a grain-growth simulation. A nicety of this microstructure is the presence of curved GBs and a network that is significantly different from those observed in Voronoi tessellated microstructures, as will be evident later. We analyze the results in terms of stresses and strains, and furthermore, in terms of statistics of dislocation activity. We compare these results to those obtained from Voronoi microstructures. Additionally, we look into differences in mechanisms and discuss these in terms of the sample characteristics, GB network and topology.

2. Methods

2.1. Sample generation

The NC structures used in this work have been generated either by Voronoi tesselation or from a grain growth simulation. In the study fully periodic boundary conditions are used to avoid surface effects. Samples, based on the Voronoi scheme, are usually generated starting from an empty simulation volume and distributing a set of points randomly. These points, or *seeds*,

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