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Non-equilibrium grain boundary structure and inelastic deformation using atomistic simulations

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ABSTRACT

Grain boundary influence on material properties becomes increasingly significant as grain size is reduced to the nanoscale. Nanostructured materials produced by severe plastic deformation techniques often contain a higher percentage of high-angle grain boundaries in a non-equilibrium or energetically metastable state. Differences in the mechanical behavior and observed deformation mechanisms are common due to deviations in grain boundary structure. Fundamental interfacial attributes such as atomic mobility and energy are affected due to a higher non-equilibrium state, which in turn affects deformation response. In this research, atomistic simulations employing a biased Monte Carlo method are used to approximate representative non-equilibrium bicrystalline grain boundaries based on an embedded atom method potential, leveraging the concept of excess free volume. An advantage of this approach is that non-equilibrium boundaries can be instantiated without the need of simulating numerous defect/grain boundary interactions. Differences in grain boundary structure and deformation response are investigated as a function of non-equilibrium state using Molecular Dynamics. A detailed comparison between copper and aluminum bicrystals is provided with regard to boundary strength, observed deformation mechanisms, and stress-assisted free volume evolution during both tensile and shear simulations.

1. Introduction

Ultrafine-grained (UFG) and nanocrystalline (NC) materials (i.e., polycrystalline materials with average grain sizes between 100 nm and 1 μm, and below 100 nm, respectively) have been extensively researched and investigated over the past 10 years due to potential improvement of many functional material properties. For example, substantial differences in strength, ductility, hardening, fracture resistance, and fatigue life compared with traditional polycrystalline materials have been measured in these materials (Gleiter, 1989; Khan et al., 2006; Meyers et al., 2006; Vinogradov et al., 1997; Zhao et al., 2008). Additional efforts have aimed at utilizing computational approaches to better understand the role of grain boundaries (GBs) and the overall mechanical behavior of NC metals Barai and Weng (2009), Capolungo et al. (2005, 2008), Farrokh and Khan (2009), Warner et al. (2006). Many investigations have further highlighted the importance of material quality through proper synthesis (Agnew et al., 2000; Khan et al., 2008). Despite these desirable characteristics, early measurements of low ductility inhibited the use of UFG and NC materials in important structural applications (Gleiter, 1989; Koch, 2003; Ma, 2003). Therefore, numerous research endeavors have aimed at increasing the strength and ductility of these materials

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