Acta Materialia 124 (2017) 588–597

Contents lists available at ScienceDirect

Acta Materialia

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

Full length article

Variability of non-Schmid effects in grain boundary dislocation nucleation criteria

Ricky D. Wyman [a], David T. Fullwood [a], Robert H. Wagoner [b], Eric R. Homer [a, *]

[a] Department of Mechanical Engineering, Brigham Young University, Provo, UT, USA
[b] Department of Materials Science and Engineering, Ohio State University, Columbus, OH, USA

ARTICLE INFO

Article history:
Received 2 September 2016
Received in revised form
20 October 2016
Accepted 2 November 2016
Available online 24 November 2016

Keywords:
Grain boundaries
Dislocation nucleation
Molecular dynamics

ABSTRACT

Grain boundary dislocation nucleation is simulated in a Nickel bicrystal with Σ21b (211)/(211) grain boundaries. Using molecular dynamics, 386 different triaxial stress states are examined for their effect on dislocation nucleation on different slip systems. The approach leads to dislocation nucleation on six of the twelve partial slip systems, enabling a study of conditions leading to nucleation. The criteria for nucleation on each of the slip systems is shown to have a linear dependence on the resolved shear, normal, and co-slip stresses, though the constants for this linear dependence are unique for each slip system. The combined nucleation criteria are used to construct a theoretical nucleation surface. The surface is reminiscent of a Mohr-Coulomb yield surface, except that in the present case the facets of the surface correspond to nucleation on different slip systems.

1. Introduction

Grain boundaries (GBs) play an important role in material strength, becoming increasingly important as grain size shrinks [1–4]. GBs act as barriers to dislocation motion and as sources and sinks for dislocations. Of primary interest in this work is the heterogeneous nucleation of dislocations, where a GB relieves local stress by emitting dislocations in one or both of the grains it separates [5–7].

Similar to homogeneous dislocation nucleation in the absence of a GB [8–10], nucleation at a GB is known to have non-Schmid stress dependence [5,11]. In particular, the critical resolved shear stress for dislocation nucleation is heavily dependent upon the resolved normal stress, where the normal stress acts perpendicular to the slip plane, as shown schematically in Fig. 1. When the resolved normal stress is compressive, it is harder for atoms to glide over each other, but when it is tensile, it is easier for atoms to glide [5].

Investigations into the conditions required for dislocation nucleation have led to a number of different conclusions. Spearot et al. applied uniaxial tension to a number of ⟨100⟩ and ⟨110⟩ tilt GBs [5]. By using a least squares fit, they built an equation to predict the uniaxial stress required to cause GB dislocation nucleation. They found that dislocation nucleation from ⟨100⟩ tilt GBs is governed primarily by the resolved normal stress while ⟨110⟩ tilt GBs are governed primarily by resolved shear stress. Beyerlein et al. proposed that dislocation nucleation is favored on slip systems well aligned with intrinsic dislocations inside the GB. The likelihood of nucleation on some slip system is then proportional to the driving stress multiplied by a structure factor quantifying the favorability of some slip systems [6]. Sangid et al. developed a method of measuring energy barriers to dislocation nucleation and found that the energy barrier for nucleation is inversely proportional to the static GB energy [12], and the nucleation event leads to a drop in GB interfacial energy [12,13]. Additional work by Spearot et al. found increased nanoporosity in a GB leads to nucleation at relatively low stresses [14], and Wang et al. found that high creep stresses can induce dislocation nucleation from GBs in nanocrystalline materials [15]. The current consensus is that GB dislocation nucleation is tied to GB structure and that resolved shear alone cannot predict when nucleation will occur.

Other factors surrounding the location of GB dislocation nucleation have also received attention. Wu et al. show that the point of nucleation within a GB is correlated with high Von Mises stress [16]. Similarly, Zhang, et al. show that nucleation tends to occur at locations with the most intense localized shear [17]. Burbery et al. correlate the nucleation location with atoms whose virial stress has a large component normal to the GB, and also note that per atom potential energy fails to predict the location of nucleation [18].

* Corresponding author.
E-mail address: eric.homer@byu.edu (E.R. Homer).

http://dx.doi.org/10.1016/j.actamat.2016.11.005
1359-6454/

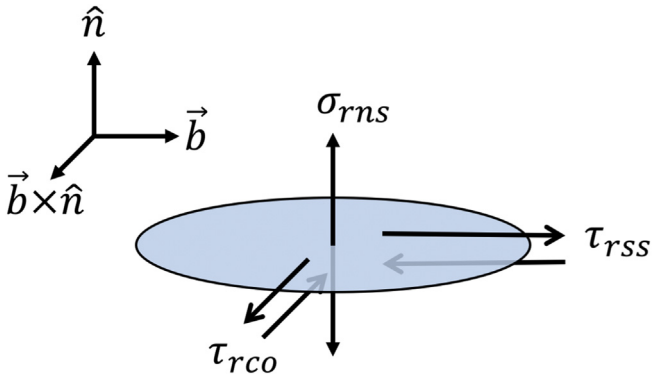

Fig. 1. Resolved shear stress (τ_{rss}), resolved normal stress (σ_{rns}) and resolved co-slip stress (τ_{rco}) shown schematically on a slip plane with normal $\hat{n}$, and τ_{rss} in the direction of the Burger's vector $\vec{b}$.

None of these observations are exclusive of the others, as all suggest nucleation occurs at locations of high stress; however, they also do not provide an overall theory on where and at what stress nucleation will occur. Such predictive capability remains an elusive goal.

In the present work, we examine a single GB under many different triaxial stress states. The approach is designed to investigate how different stress states influence dislocation nucleation on different slip systems. Using stress states measured near the GB at the time nucleation occurs, we are able to determine the relative influence of shear, normal, and co-slip stresses on GB dislocation nucleation. The analysis produces unique nucleation criteria for different slip systems that can combine to give a nucleation surface that predicts dislocation nucleation. The significance of these results are discussed in the context of the literature.

2. Methodology

2.1. Molecular dynamics simulations

The present work simulates an atomistic model of a Σ21b [211] 44.415° symmetric twist Nickel GB subjected to a range of triaxial stress states to measure the conditions surrounding GB dislocation nucleation. The GB has (211) boundary planes in both crystals and can also be described as a [421] 180° symmetric tilt GB. The work focuses on one of two GBs in a fully periodic bicrystal. The bicrystal is shown in Fig. 2 with atoms colored by their common neighbor analysis (CNA) value [19]. The smaller middle grain, grain A, is 126 Å wide, the larger outer grain, grain B, is 234 Å wide. The dimensions in the *y* and *z* directions of the orthogonal simulation cell are 33 Å and 32 Å, respectively. In total, the system contains 31,500 atoms. The bicrystal is derived from one of the computed GBs prepared by Olmsted et al. [20,21]. Molecular dynamics is performed with LAMMPS [22] utilizing GPU accelerated hardware [23–25] with the Foiles-Hoyt Nickel embedded atom potential [26]. Visualization of the bicrystal is performed with OVITO [27]. The bicrystal is simulated at 0.1 K to minimize the contributions of thermal energy, as has been done in other work [11]. The bicrystal is equilibrated at the desired temperature and zero pressure for 100 ps using an NPT ensemble and the Nosé-Hoover thermostat [28,29].

To achieve the range of desired triaxial stress states to be applied to the simulation cell, each individual stress state is specified by a unit vector, λ. Each component of this λ vector represents the relative stress magnitude and sign in the $\hat{x}$, $\hat{y}$, and $\hat{z}$ dimensions, respectively. The λ vector is then defined as

$$\lambda = \frac{\left[\sigma_x, \sigma_y, \sigma_z\right]}{\sqrt{\sigma_x^2 + \sigma_y^2 + \sigma_z^2}} \tag{1}$$

To examine the full range of triaxial stress states, we select 386 unique points approximately equidistributed about a unit sphere [30] where the Cartesian coordinates of each point on the sphere gives the values for the λ unit vectors.

For each λ vector, molecular dynamics is used to simulate a triaxial stress test on the bicrystal with the intention of inducing GB dislocation nucleation. The Nosé-Hoover thermostat is again used to maintain the desired temperature and ramp the applied σ_x, σ_y, and σ_z stresses in their corresponding directions from 0 GPa such that their geometric norm grows at a rate of 100 MPa/ps. The barostat ensures that the relative pressures in the three directions conform to the λ vector for the target triaxial stress state. The simulation is terminated shortly after plasticity occurs, which is usually associated with GB dislocation nucleation.

2.2. Analysis methodology

To analyze the conditions leading to GB dislocation nucleation over the range of triaxial stress states, each simulation must first be analyzed to determine the slip system on which dislocation nucleation occurs, and the resolved stresses associated with that nucleation event. As noted above, the work focuses on only one of the two GBs. Furthermore, because the analysis for nucleation from that GB into grains A and B are similar, most of the analysis focuses on nucleation into grain A, though some results for grain B are also included to show similarity.

For the Nickel GB analyzed here, partial dislocations with a trailing stacking fault are the primary dislocation nucleation event observed, so dislocation nucleation is analyzed in terms of the twelve $\{111\}\langle 11\bar{2}\rangle$ partial dislocation slip systems. The stacking faults simplify the identification of the slip systems, because the atoms are easily identified by their CNA value. The slip plane is found by fitting a plane to the slipped atoms, while the slip direction is determined by examining the slip vector [31] of these same atoms.

In this work, the stresses that lead to nucleation are analyzed based on the local stress near the GB. The global stress is not used because it can differ significantly from the local stress where nucleation actually occurs. The stress exactly in the GB is also not used because the GB itself has a complicated stress state due to atomic disorder as well as the anisotropy caused by the differing orientations of the grain on either side. Instead, the local stress is determined by averaging the virial stress [32] of all atoms between

Fig. 2. The Σ21b [211] 44.415° symmetric twist Nickel GBs used in this work. Atoms are colored by their common neighbor analysis (CNA) value (FCC = blue, HCP = turquoise, Undefined = red). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)