

# Atomistic Simulations of Dislocation Nucleation

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## ABSTRACT

The objective of this research is to use atomistic simulations to investigate dislocation nucleation from asymmetric tilt grain boundaries in FCC copper and aluminum. We use a 3D periodic bicrystal configuration to investigate how grain boundary degrees of freedom impact both the boundary structure and dislocation nucleation in symmetric and asymmetric tilt boundaries. Simulation results show that dislocation nucleation from asymmetric tilt grain boundaries requires understanding of the structure and faceting of these boundaries. Deformation simulations of single crystals and grain boundaries under uniaxial tension and compression show entirely different nucleation mechanisms, i.e., nucleation of full dislocations in copper from the grain boundary under compression. Analysis of the resolved stresses shows that the resolved stress normal to the slip plane on which the dislocation nucleates plays an integral role in dislocation nucleation for both single crystals and interfaces.

## 1.0 Introduction

Enhanced functional properties in materials containing nanometer length scales has also fueled the desire to better understand the mechanical properties of these materials. In particular, nanocrystalline materials have attracted much interest due to their increased grain boundary fraction which contributes to changes in the plastic deformation mechanisms of nanocrystalline metals, *i.e.*, grain boundary sliding and grain boundary dislocation nucleation and emission [1-3]. Additionally, recent mechanics experiments in nanopillars attempt to probe the intrinsic dislocation behavior at these scales [4, 5]. However, designing mechanics experiments at this scale to investigate dislocation-based mechanisms in grain boundaries and single crystals have many challenges; an alternative is the use of computational simulations. Atomistic simulations can serve as an effective tool for probing the mechanical properties and mechanisms of materials at these length scales. In this work, atomistic simulations are used to investigate dislocation nucleation from grain boundaries in face-centered cubic aluminum and copper [6, 7]. This research primarily focuses on asymmetric tilt grain boundaries and has three main components, the results of which are presented in Sections 3.1, 3.2 and 3.3.

First, this research uses molecular statics simulations of the structure and energy of these faceted, dissociated grain boundary structures to show that  $\Sigma 3$  asymmetric boundaries can be decomposed into the structural units of the  $\Sigma 3$  symmetric tilt grain boundaries [8, 9], *i.e.*, the coherent twin and the  $\Sigma 3(112)$  boundary. Moreover, the energy for all  $\Sigma 3$  asymmetric boundaries is predicted

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with only the energies of the  $\Sigma 3$  symmetric boundaries and the inclination angle [8]. Understanding the structure of these boundaries provides insight into dislocation nucleation from these boundaries. Further work into the structure and energy of other low order  $\Sigma$  asymmetric boundaries [10] and the spatial distribution of free volume within the grain boundaries [11] also provides insight into dislocation nucleation mechanisms.

Second, this research uses molecular dynamics deformation simulations with uniaxial tension applied perpendicular to these boundaries to show that the dislocation nucleation mechanisms in  $\Sigma 3$  asymmetric boundaries are highly dependent on the faceted, dissociated structure [12]. Grain boundary dislocation sources can act in different manners depending on the specific dislocation content of the boundary [13]. Furthermore, simulations under uniaxial tension and uniaxial compression show the tension-compression asymmetry in the nucleation stress [14] and the nucleation of the trailing partial dislocation in copper [15, 16].

Third, this research explores the development of simulation-based models that incorporate the resolved stress components on the slip system of dislocation nucleation to predict the atomic stress required for dislocation nucleation from single crystals and grain boundaries [17]. Single crystal simulations of homogeneous dislocation nucleation help define the role of lattice orientation on the nucleation stress for grain boundaries [16, 18]. The resolved stress normal to the slip plane on which the dislocation nucleates plays an integral role in the dislocation nucleation stress and related mechanisms [16, 18]. Additional work investigating the role of thermal activation on dislocation nucleation has shown activation volumes of  $\sim 1 b^3$  and activation energies of  $\sim 0.30$  eV for 300 K bicrystal and single crystal simulations [7, 16]. This paper discusses various aspects of this work, the synthesis of which has provided improved understanding of *homogeneous* and *heterogeneous* dislocation nucleation in single crystals and grain boundaries, respectively.

## 2.0 Methods

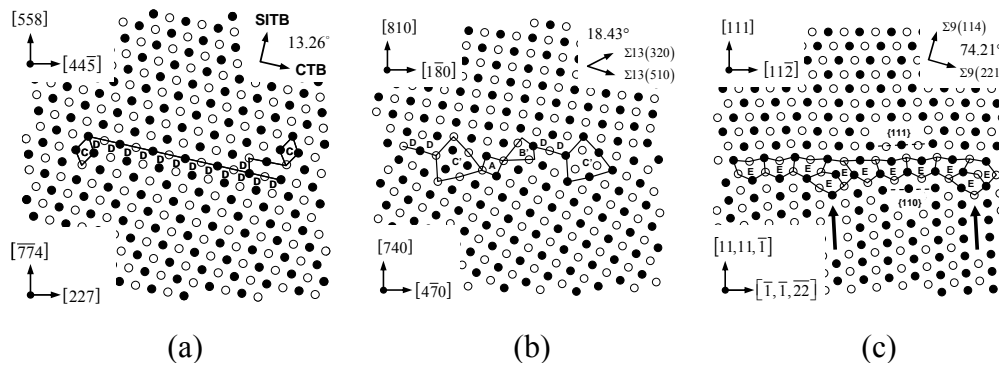
A parallel molecular dynamics code (Warp [19]) was used to generate the grain boundary structures and deform the bicrystal and single crystal configurations. The Mishin et al. [20] embedded-atom method potential for Cu was primarily used because of its accurate description of the stable and unstable stacking fault energies. The grain boundary structures were generated by using a large number of starting configurations with a nonlinear conjugate gradient technique to locate the minimum energy 0 K structure [8-11]. The single crystal and bicrystal atomic configurations were deformed in a 3D periodic computational cell under an applied uniaxial tensile load at a constant strain rate of  $10^9 \text{ s}^{-1}$ , as in Refs. [12-16]. Moreover, recent calculations by Spearot et al. [21] show that the dislocation nucleation stress in single crystal calculations is not greatly affected by the strain rate, as in some nanocrystalline simulations [22]. For mechanical properties, the virial stress was used to calculate the stress required for dislocation nucleation.

### 3.0 Results – Atomistic simulations of dislocation nucleation

Analyzing the influence of GB character on dislocation nucleation in molecular dynamics simulations of three-dimensional (3D) nanocrystalline materials is very complex. The combined tilt and twist character of grain boundaries and the inclination of the grain boundary plane with respect to the tensile axis complicates the analysis of the role of specific GB structures in nanocrystalline simulations. Additionally, different boundaries may nucleate and emit dislocations at different stresses; it becomes very difficult to separate out the individual effects of GB structure on dislocation nucleation. This motivated us to use bicrystal simulations to study how specific GBs impact dislocation nucleation mechanisms. In this work, previous bicrystal simulations of dislocation nucleation in symmetric tilt grain boundaries [23, 24] were extended to the structure-`dislocation nucleation' relationships of asymmetric tilt grain boundaries. There are a multitude of research questions that persist pertaining to the structure of asymmetrical grain boundaries and their dislocation nucleation behavior. The following subsections highlight some work in this area.

#### 3.1 Grain boundary structure, energy, and free volume

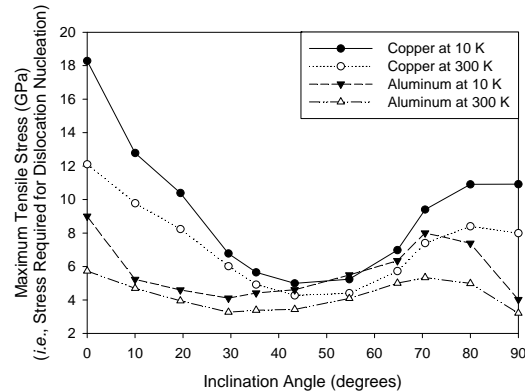
The grain boundary structure, energy, and free volume were calculated for several low-order coincident site lattice systems [8-10]:  $\Sigma 3$ ,  $\Sigma 5$ ,  $\Sigma 9$ ,  $\Sigma 11$ , and  $\Sigma 13$ . Figure 1 shows a few examples of the structures obtained. Structural units -- clusters of atoms representing grain boundary dislocation content -- were outlined for boundary atoms with a high degree of non-centrosymmetry. First, some boundaries exhibit faceting at the nanoscale, i.e., there are reoccurring structural units that are inclined with respect to the mean boundary plane. This is evident for the  $\Sigma 3$ ,  $\Sigma 5$ , and  $\Sigma 13$  boundaries in Cu and Al (e.g., Fig. 1a and 1b). In these cases, the asymmetric boundary can often be decomposed into the structural units of the symmetric tilt grain boundaries of the same  $\Sigma$ -value. However, some boundaries rearrange such that the boundary atoms align along low index planes of low energy, as in Fig. 1c. In many cases, there is also a definitive relationship between the asymmetrical grain boundary structure and the boundary energy [10].



**Figure 1.** Calculated asymmetric tilt grain boundary structures for (a)  $\Sigma 3$ , (b)  $\Sigma 13$  and (c)  $\Sigma 9$  boundaries in Cu [8-10]. Black and white atoms represent atoms on different  $\{110\}$  planes.

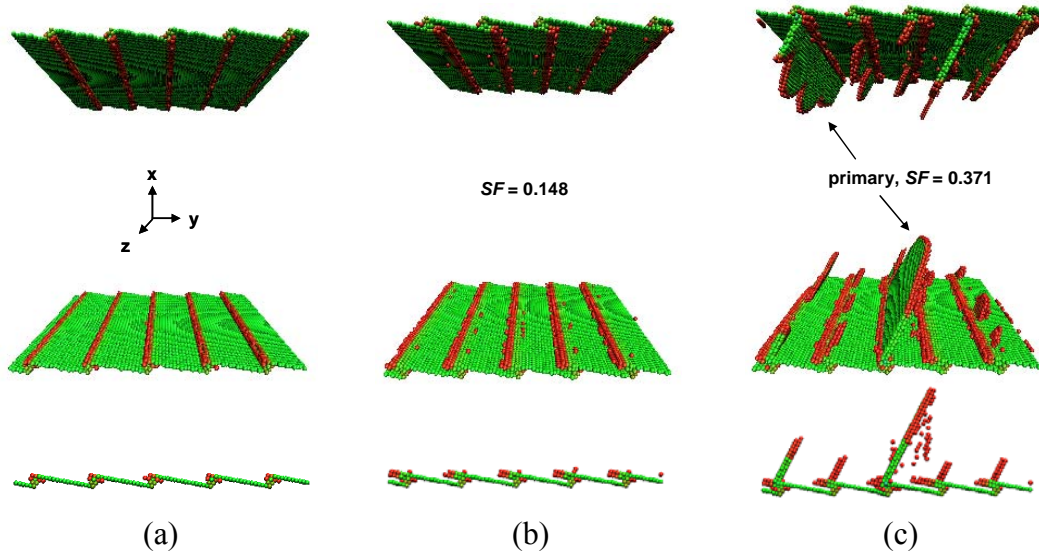
### 3.2 Dislocation nucleation stresses and mechanisms

The stress required to nucleate dislocations is linked to the grain boundary structure and can assume very different values depending on the grain boundary and surrounding crystal lattice character. Figure 2 shows how the dislocation nucleation stress evolves as a function of the inclination angle for  $\Sigma 3$  boundaries, where the inclination angle refers to the degree of rotation of the boundary plane from the coherent twin about the  $\langle 110 \rangle$  tilt axis. All grain boundaries in this plot have the same misorientation angle, but very different nucleation stresses. For copper, the variation in dislocation nucleation stresses can be explained by the different structures and nucleation mechanisms in these boundaries.



**Figure 2.** Graph that shows how the dislocation nucleation stress evolves as a function of inclination angle for  $\Sigma 3$  asymmetric tilt grain boundaries [12].

The dislocation nucleation mechanism helps explain the relative magnitude of the stress required to nucleate dislocations from the boundary. The grain boundary structure evolves as a function of the load applied perpendicular to the boundary. In some boundaries (inclination angles  $\sim 45^\circ$  in Fig. 2), the dislocation is nucleated and emitted on the same  $\{111\}$  plane that boundary dislocations dissociated onto, which requires a relatively low dislocation nucleation stress. Figure 3 shows an example of the evolution of structure for a  $\Sigma 3$  asymmetric boundary with an inclination angle of  $10.02^\circ$  (similar structure to Fig. 1a), which requires a relatively high dislocation nucleation stress. In this case, grain boundary dislocations initially dissociate into the lattice on one  $\{111\}$  plane, but the partial dislocations that are emitted from the boundary lie on a different  $\{111\}$  slip plane with a higher Schmid factor (resolved shear stress). But why doesn't the partial dislocation dissociate and emit on the maximum Schmid factor  $\{111\}$  slip plane from the onset of deformation? The initial dissociation of a dislocation on a low Schmid factor  $\{111\}$  plane emphasizes that the dislocation content and their arrangement within the boundary plays an important role in the dislocation nucleation process. Indeed, Tschopp and McDowell [12] show that the ease of dislocation nucleation in  $\Sigma 3$  asymmetric boundaries depends greatly on how the initial dislocation content manifests itself as facets and structural units, and how this dislocation content relates to  $\{111\}$  slip planes in adjoining crystal lattices. Also, note that partial dislocations are only emitted into one lattice and that this lattice does not necessarily contain the  $\{111\}$  slip plane with the highest resolved shear stress. Again, this emphasizes that the boundary dislocation arrangement plays a critical role in dislocation nucleation.

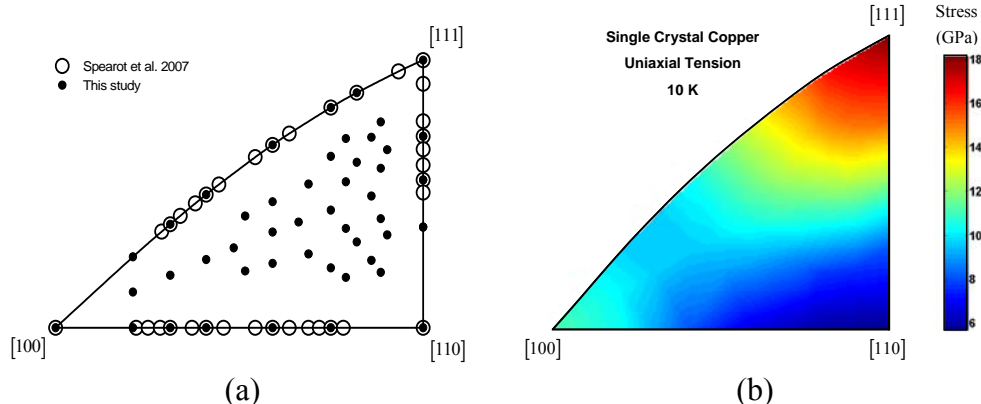


**Figure 3.** Evolution of boundary structure under uniaxial tensile deformation of  $\Sigma 3$  asymmetric tilt boundary at 10 K [12]. Only atoms in a non-centrosymmetric environment are shown.

### 3.3 Results – Dislocation nucleation model

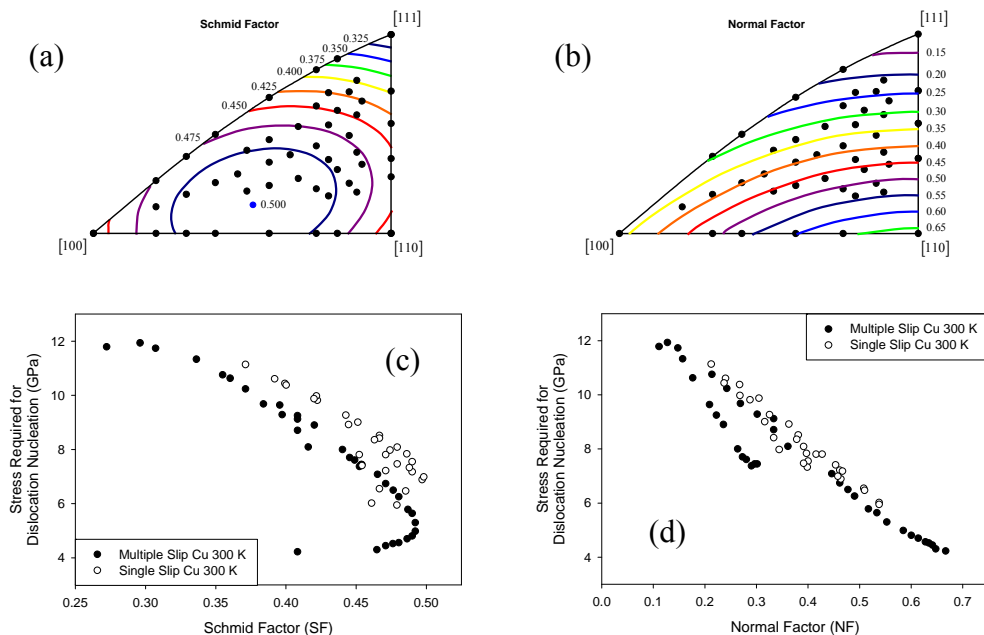
Investigating how grain boundary degrees of freedom affect the stress required to nucleate dislocations from the boundary can provide further quantitative insight into dislocation nucleation. Spearot et al. [17] formulated a model that correlates the calculated dislocation nucleation stresses with continuum parameters related to resolved stresses and interface structure. Atomistic simulations from this work indicated that the orientation of the opposing lattice regions and the presence of certain structural units were two critical attributes that affected the dislocation nucleation stress. In particular, though, there was a need to better understand how lattice orientation affects *homogeneous* dislocation nucleation in single crystals prior to formulating a model for *heterogeneous* dislocation nucleation in grain boundaries. Here we highlight some work pertaining to dislocation nucleation in single crystals.

The influence of the surrounding crystal lattice on dislocation nucleation was calculated by deforming three-dimensional (3D) periodic single crystal configurations until homogeneous dislocation nucleation occurs. Tschopp et al. [18] used 47 different loading orientations to examine how the homogeneous nucleation stress varied in single crystal copper under uniaxial tension. The crystal orientations are shown in Fig. 4a. A contour plot of the dislocation nucleation stresses calculated as a function of crystallographic orientation over the entire stereographic triangle is shown in Fig. 4b. Interestingly, the dislocation nucleation stress does not directly correlate with the Schmid factor, *i.e.*, dislocation nucleation requires a different formulation than dislocation motion. This can be easily observed from Fig. 4b by comparing the contours at the [100] and [110] loading axes; the Schmid factor for both directions is equal (0.408).



**Figure 4.** (a) Uniaxial loading orientations for single crystal Cu [17, 18]. (b) Contour plot of calculated stresses required for homogeneous dislocation nucleation as a function of loading orientation [18].

Figure 5a and 5b shows the change in the Schmid factor (resolved shear stress in the direction of slip) and the normal factor (resolved normal stress) as a function of crystallographic orientation. The Schmid factor and normal factor represent the direction cosines term required to resolve the uniaxial tensile stress onto the  $\{111\}$  slip plane into the direction of slip and normal to the  $\{111\}$  plane, respectively. Consequently, a high Schmid (normal) factor results in a higher resolved shear (normal) stress, and so on. Figure 5c shows that the stress required for dislocation nucleation increases as the Schmid factor decreases; Figure 5d shows that the dislocation nucleation stress increases as the normal factor decreases as well. Both relations show nonlinear behavior, though.



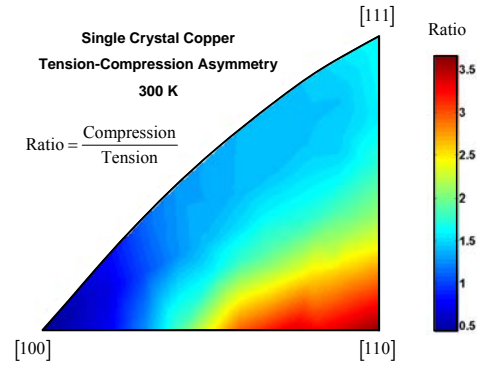
**Figure 5.** (a) Schmid factor and (b) normal factor as a function of crystallographic orientation. The dislocation nucleation stress as a function of the (c) Schmid factor and (d) normal factor for single slip and multiple slip orientations [17].

The calculated nucleation stresses are then modeled by assuming that dislocation nucleation occurs when a combination of the Schmid resolved shear stress ( $\sigma_{SF}$ ) and the resolved normal stress ( $\sigma_{NF}$ ) reach some pre-determined nucleation stress magnitude, *i.e.*,  $\tau_{\text{nucleation}} = \mu_s \sigma_{SF} + \mu_n \sigma_{NF}$ . In this manner, a coupling between tensile and resolved stresses is allowed through weighting coefficients,  $\mu_s$  and  $\mu_n$ . Assuming that  $\tau_{\text{nucleation}} = 2.16$  GPa [25], the critical stress  $\sigma$  can be calculated for a single crystal lattice, *i.e.*,

$$\sigma = \frac{\tau_{\text{nucleation}}}{\mu_s SF + \mu_n NF} \quad (1)$$

This formulation has been additionally modified for loading orientations in the stereographic triangle where dislocation nucleation is more strongly influenced by either the resolved shear stress or resolved normal stress [18]. For some orientations, the dislocation nucleation stress is strongly correlated with the resolved stress normal to the  $\{111\}$  slip plane. Interestingly, the resolved normal stress is also of great interest in ideal shear strength calculations [25, 26].

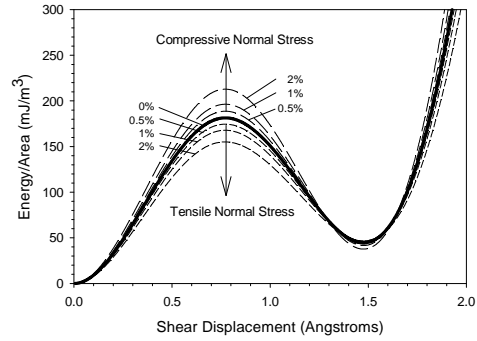
The strong role of the resolved normal stress has led to further studies that investigate the difference in dislocation nucleation response between uniaxial tension and compression. Figure 6 shows that there is a large tension-compression asymmetry in dislocation nucleation stresses for single crystals. While the resolved shear stress does not change between tension and compression, the resolved normal stress does – in tension, it is tensile, and in compression, it is compressive. For most orientations (other than  $[100]$ ), this results in much higher dislocation nucleation stresses required in compression. The resolved normal stress acts as an interatomic friction between the  $\{111\}$  planes; in compression, compressive normal stresses provide more friction to the  $\{111\}$  planes, necessitating higher stresses to overcome this friction and nucleate dislocations, and in tension, vice versa.



**Figure 6.** Tension-compression asymmetry in dislocation nucleation stresses for single crystal copper [14, 16].

The effect of the normal stress under tension and compression also affects the dislocation nucleation mechanisms. In both grain boundaries [15] and single crystal [16] configurations for copper, only partial dislocations are nucleated under uniaxial tensile stresses. However, under uniaxial compression of the same grain boundary and single crystal configurations, full dislocations are often nucleated. This implies that the nucleation of the second partial dislocation in nanocrystalline systems may be related to the resolved normal stress [15, 16].

The nucleation of the trailing partial dislocation is often associated with arguments based on the unstable and stable stacking fault energy [27, 28]. Figure 7 shows the influence of the resolved normal stress on the stacking fault energy curve in copper. The unstable stacking fault energy shifts in a manner that is contrary to what would be expected based on what is observed in our atomistic simulations; increasing the unstable stacking fault energy in compression should result in a larger energy barrier to nucleating a trailing partial dislocation. Again, the resolved normal stress has a critical role in the physics involved with dislocation nucleation. Further work is needed to fully understand the calculated mechanistic differences between tension and compression.



**Figure 7.** Influence of the resolved normal stress on the stacking fault energy curve in copper [16].

Last, an equally important aspect of a dislocation nucleation model is the ability to account for thermal activation. The present work uses MD simulations to construct an activation volume and activation energy-based approach for thermally-assisted dislocation nucleation [7, 16]. We have found reasonable agreement with calculated nucleation stresses using activation volumes of  $\sim 1 \text{ b}^3$  and activation energies of  $\sim 0.30 \text{ eV}$  for both our single crystal and bicrystal simulations. Interestingly, Schuh et al. [29] measured activation volumes of  $\sim 1 \text{ b}^3$  and activation energies of  $\sim 0.3 \text{ eV}$  from nanoindentation experiments on platinum at various temperatures, very close to the values computed by Tschopp and McDowell [16] for pure Cu.

#### 4.0 Conclusions

In this work, atomistic simulations are used to explore the influence of grain boundary degrees of freedom on dislocation nucleation from asymmetric tilt grain boundaries. A full understanding of dislocation nucleation from grain boundaries requires knowledge of the grain boundary structure and its relationship with dislocation mechanics and mechanisms. Single crystal simulations shed further light on the role of crystal orientation in *homogeneous* dislocation nucleation and *heterogeneous* nucleation from grain boundaries. An important finding of this work is how the non-Schmid normal stress influences dislocation nucleation.

#### Acknowledgments

This material is based upon work supported under an NSF Graduate Research Fellowship (M.A.T.). This work was partially supported by the NCSA under DMR060019N and utilized Cobalt. D.L.M. is grateful for the additional support of this work by the Carter N. Paden, Jr. Distinguished Chair in Metals Processing.



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