

Tension-Compression Asymmetry in Homogeneous Dislocation Nucleation in Single Crystal Copper

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This letter addresses the dependence of homogeneous dislocation nucleation on the crystallographic orientation of pure copper under uniaxial tension and compression. Molecular dynamics simulation results with an embedded-atom method potential show that the stress required for homogeneous dislocation nucleation is highly dependent on the crystallographic orientation and the uniaxial loading conditions; certain orientations require a higher stress in compression (*e.g.*, [110] and [111]) and other orientations require a higher stress in tension ([100]). Furthermore, the resolved shear stress in the slip direction is unable to completely capture the dependence of homogeneous dislocation nucleation on crystal orientation and uniaxial loading conditions.

As material microstructure progresses towards nanometer scale dimensions to achieve enhanced functional properties, understanding the mechanical properties becomes vital. Of particular interest is the asymmetry in dislocation nucleation stress between tension and compression. Atomistic simulations provide an effective tool for analyzing this tension-compression asymmetry. For example, Diao *et al.* [1] have shown that the yield strength asymmetry in Au nanowires for the [100] and [111] orientations are due to surface-induced internal stresses. Tomar and Zhou [2] related the yield strength asymmetry in nanocrystalline α -Fe₂O₃-fcc Al composites to differences in grain boundary sliding behavior. Lund *et al.* [3, 4] have shown that nanocrystalline Ni has higher yield and flow stresses in compression than in tension (both uniaxial and biaxial simulations); these results suggest a similar atomic-level mechanism controls yield in both fcc Ni and metallic glasses [5]. Cheng *et al.* [6] propose a pressure-dependent analytical model that predicts the observed tension/compression asymmetry of the yield strength in nanocrystalline Fe, Cu, and Al. While these studies focused on inelastic deformation due to heterogeneities at the nanoscale, the influence of crystal orientation on dislocation nucleation in the *absence* of heterogeneities is also vital to a full understanding of inelasticity at the nanoscale. In this letter, we analyze (i) the asymmetry in the tensile and compressive stress values required to homogeneously nucleate partial dislocations in single crystal copper and (ii) how well the conventional Schmid factor for dislocation motion describes dislocation nucleation within the single crystal models.

A parallel molecular dynamics (MD) code (WARP [7]) was used to deform the single crystal atomistic models in

uniaxial tension and compression. The single crystal configuration was first equilibrated at 300 K for 10 ps in the isobaric-isothermal (NPT) ensemble [8] with zero applied pressure. Next, the configuration was deformed in either uniaxial tension or compression at a constant strain rate of 10^9 s^{-1} with a stress-free condition for the other two boundaries [9, 10]. We employ an embedded-atom method [11] potential for Cu [12] in this study. Copper is an ideal fcc material that exhibits weak bond directionality [13], admitting accurate characterization by the non-directional nature of the embedded-atom method. The Mishin potential provides a relatively accurate description of both the unstable (γ_{usf}) and stable (γ_{sf}) stacking fault energies compared to density functional theory calculations [14], which is important for atomistic simulations of dislocation nucleation.

For mechanical properties, the system stress was calculated using the virial definition without the kinetic portion [15], as used in previous MD simulations which investigated length scale effects on yield [16]. Throughout this work, the **stress required for homogeneous dislocation nucleation** is defined as the maximum uniaxial tensile/compressive stress. Visualizing the deformation of selected loading axis orientations with the centrosymmetry parameter [17] has shown that dislocations are nucleated at a strain very close to the maximum stress for all single crystal models. In some cases, dislocations appeared to nucleate slightly before the maximum stress is reached ($< 1.0\%$ below the maximum stress). However, in light of the difficulty of visually ascertaining exactly when the dislocation nucleates (*i.e.*, how many spatially clustered, disordered atoms on the slip plane constitute a dislocation?), the maximum tensile/compressive stress accurately indicates the stress required to homogeneously nucleate a partial dislocation loop in a single crystal.

A 3D periodic computational cell was used to investigate *homogeneous* dislocation nucleation in single crystal Cu under uniaxial loading at a constant strain rate. A minimum length of 16 nm in all directions (*i.e.*, 352,800-

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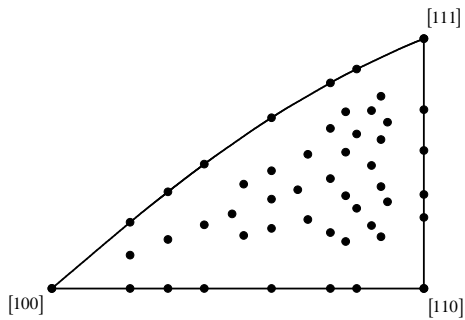


FIG. 1: Stereographic triangle showing the 49 uniaxial loading axis orientations investigated in the single crystal deformation simulations.

842,400 atoms) was chosen to properly enforce the 3D periodic boundary conditions. Although not explicitly shown, increasing the simulation cell size further has little effect on the dislocation nucleation stress (*i.e.*, an error of $\leq 0.8\%$ for the maximum tensile stress of a 16^3 nm^3 cell compared to a 24^3 nm^3 cell with a $[321]$ axis).

Figure 1 shows the 49 loading axis orientations examined within the basic stereographic triangle with $[100]$, $[110]$, and $[111]$ vertices. The plot axes are the longitude and latitude values for each loading axis orientation [18]. Each single crystal model was deformed under uniaxial tension and compression at 300 K. The expected slip system (maximum Schmid factor) is the $(11\bar{1})[101]$ slip system for all axis orientations on the interior of the $[100]$ - $[110]$ - $[111]$ triangle, while all axis orientations on the boundary of the stereographic triangle have at least two active slip systems. The $[110]$, $[111]$, and $[100]$ vertices have 4, 6, and 8 active slip systems, respectively.

The stress required for homogeneous dislocation nucleation is calculated for all axis orientations. Figure 2 shows contour plots of the stress required for dislocation nucleation as a function of the loading axis orientation on the stereographic triangle for uniaxial (a) tension and (b) compression at 300 K. All intermediate tensile axis orientations in the stereographic triangle were obtained through linear interpolation. For both tension and compression, the $[111]$ axis requires the largest stress for dislocation nucleation. However, there is a distinctly different orientation dependence of the stress required for dislocation nucleation in tension and compression. For example, notice that the $[110]$ axis requires the lowest stress for dislocation nucleation in tension and the $[100]$ axis requires the lowest stress in compression.

Figure 3 shows the ratio of the stress required for homogeneous dislocation nucleation under compression to that in tension as a function of the loading axis orientation of single crystal copper. A ratio greater than unity signifies that homogeneous dislocation nucleation requires a higher stress in compression than in tension, and vice versa. Most orientations within the stereographic triangle require a higher stress in uniaxial *com-*

pression to nucleate dislocations; the $[110]$ axis has the largest ratio of 3.69 (15.58 GPa in compression/4.23 GPa in tension). Interestingly, not all orientations display this trend. Figure 3 also shows that some axis orientations require a greater stress in uniaxial *tension* than uniaxial compression. Specifically, the $[100]$ axis has the lowest ratio of 0.41 (3.71 GPa/9.12 GPa), showing a much greater propensity to homogeneously nucleate partial dislocations under an applied uniaxial compressive stress. Assuming a random distribution of crystal orientations in nanocrystalline materials, the influence of crystal orientation alone suggests that nanocrystalline materials should have a higher yield strength in compression than tension, agreeing with previous simulations and analytical models of nanocrystalline fcc metals [3, 6], metallic glasses [5], and nanocrystalline $\alpha\text{-Fe}_2\text{O}_3$ -fcc Al composites [2].

The glide of dislocations in fcc crystals is commonly observed to obey Schmid's law, whereby the applied stress is resolved onto the slip planes in the direction of slip. The relationship between homogeneous dislocation nucleation and the Schmid factor is unclear, though. Figure 4 shows how the Schmid factor (SF) changes as a function of the crystal orientation with respect to the uniaxial loading axis. The maximum $SF = 0.5$, occurs in the interior of the stereographic triangle and the minimum Schmid factor, $SF = 0.272$, occurs for the $[111]$ orientation. The maximum stress required in tension and com-

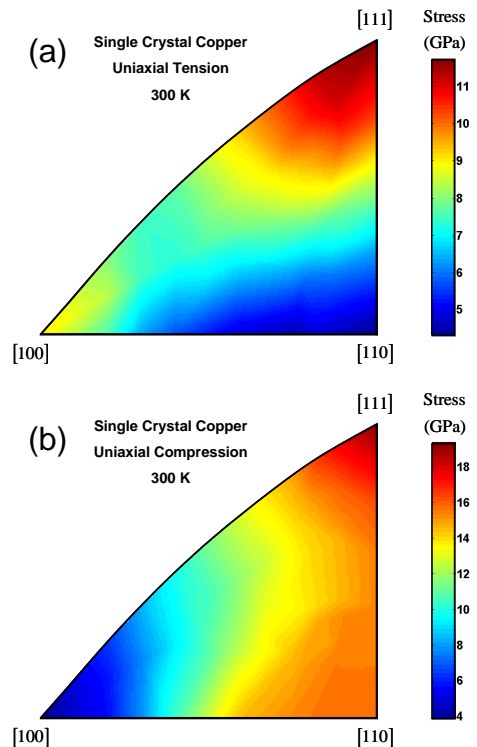


FIG. 2: (a) Tensile and (b) compressive stress required for homogeneous dislocation nucleation as a function of the loading axis orientation for single crystal models at 300 K.

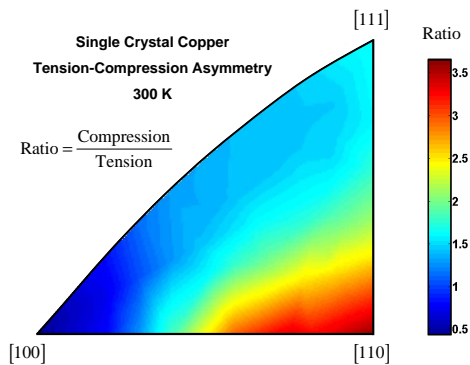


FIG. 3: The tension-compression asymmetry for homogeneous dislocation nucleation in single crystals as a function of the axis orientation at 300 K. The tension-compression asymmetry is rendered by plotting the ratio of the stress required for homogeneous dislocation nucleation in uniaxial compression to that in uniaxial tension.

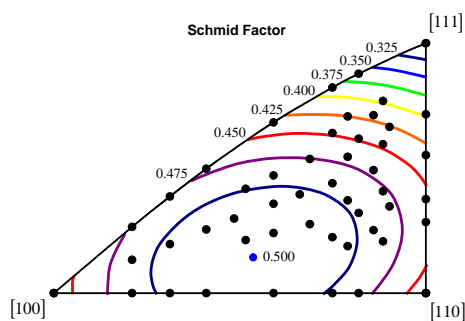


FIG. 4: (color online) Crystallographic orientation dependence of the Schmid factor (SF) for fcc crystals.

pression ([111]) corresponds to the minimum SF value, as expected. In general, calculations have shown that

the stress required for dislocation nucleation does not directly correspond to the SF for all orientations, though [19]. This can be observed from the contour differences between Fig. 2 and Fig. 4. The lack of the dependence of homogeneous dislocation nucleation on SF indicates that non-Schmid stresses are required to describe the dislocation nucleation process in single crystals. This result agrees with the *ab initio* calculations of Ogata *et al.* [13], which have shown that compressive stress components acting normal to the slip plane (non-Schmid stresses) can affect the critical resolved shear stress in Cu and Al.

In conclusion, we have utilized 49 single crystal orientations (Fig. 1) in a molecular dynamics framework to show a tension-compression asymmetry in homogeneous dislocation nucleation stress in pure copper under uniaxial loading. The stress required for homogeneous dislocation nucleation has a large orientation dependence in both uniaxial tension and compression, as shown in Fig. 2. Figure 3 shows that most orientations in the stereographic triangle require a higher stress in compression than in tension (*e.g.*, [110] and [111]), while other orientations require a higher stress in tension ([100]). Furthermore, Fig. 4 and previous calculations [19] indicate that the resolved shear stress in the direction of slip is unable to capture the influence of crystal orientation on dislocation nucleation. These observations not only indicate the importance of single crystal orientation and loading conditions on *homogeneous* dislocation nucleation but may also help in our understanding of the combined behavior of lattice orientation and heterogeneities on inelasticity at the nanoscale as well.

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