

# Dislocation Nucleation in $\Sigma 3$ Asymmetric Tilt Grain Boundaries

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## Abstract

Atomistic simulations were used to investigate dislocation nucleation from  $\Sigma 3$  asymmetric (inclined) tilt grain boundaries under uniaxial tension applied perpendicular to the boundary. Molecular dynamics was employed based on embedded atom method potentials for Cu and Al at 10 K and 300 K. Results include the grain boundary structure and energy, along with mechanical properties and mechanisms associated with dislocation nucleation from these  $\Sigma 3$  boundaries. The stress and work required for dislocation nucleation are calculated along with elastic stiffness of the bicrystal configurations, exploring the change in response as a function of inclination angle. Analyses of dislocation nucleation mechanisms for asymmetric  $\Sigma 3$  boundaries in Cu show that dislocation nucleation is preceded by dislocation dissociation from the boundary. Then, dislocations preferentially nucleate in only one crystal on the maximum Schmid factor slip plane(s) for that crystal. However, this crystal is not simply predicted based on either the Schmid or non-Schmid factors. The synthesis of these results provides a better understanding of the dislocation nucleation process in these faceted, dissociated grain boundaries.

*Key words:* Dislocations, Grain boundaries, Polycrystalline Material, Molecular Dynamics

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