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Entropic stabilization of nanoscale voids in materials under tension DANNY PEREZ, ARTHUR F. VOTER, TIMOTHY C. GERMANN, Theoretical Division T-1, Los Alamos National Laboratory, Los Alamos, NM — While preexisting defects are known to act as nucleation sites for plastic deformation in strained materials, the kinetics of the early stages of plastic yield are still poorly understood. We use a wide range of atomistic simulation techniques (molecular dynamics, accelerated molecular dynamics, umbrella sampling, etc) to investigate the kinetics of plastic yield around small nanoscale voids in copper under uniaxial tensile strain. We demonstrate that, at finite temperatures, these voids are stabilized by strong entropic effects and show that their lifetime is significant even when the static mechanical instability limit is exceeded. This stabilization phenomenon dramatically affects the yield kinetics: the lifetime of the voids is seen to increase with increasing temperature, in contrast with the usual thermally-activated behavior. Even accounting for thermal activation, very small voids prove to be extremely inefficient nucleation sites for plasticity.

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