

Thermally-Activated Plasticity at the Atomic Scale

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Plasticity and fracture are strongly affected when dislocation glide or nucleation are thermally-activated. Such processes are difficult to study from atomic-scale simulations because they are stochastic with waiting times that rapidly exceed the simulation time when the temperature decreases. Here, we review recent results obtained by a combination of molecular static (MS) and dynamic (MD) simulations. We consider the thermally-activated glide of dislocations in high Peierls stress crystals where the dislocation velocity is expected to depend exponentially on the kink-pair activation enthalpy. We verify the validity of this relation and compute the pre-exponential factor by comparing MD simulations to static Nudged Elastic Band method calculations of the activation enthalpy. The activation enthalpy versus applied stress curve is analyzed using a line tension model of a dislocation moving on a stress-dependent substrate potential. Results are discussed and compared to experimental data on the temperature dependence of the flow stress.