Graduate Student Research Seminar

Fall 2024

Effect of Entropy and Langevin Friction on the Dislocation Glide Mechanisms

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Monday, November 25th
3:00 pm (EST) – 132 Fluor Daniel Building

Abstract

Thermal activation of dislocations is critical for predicting the mechanical response of materials under common experimental conditions. According to transition state theory (TST), the rate for the system to overcome free energy barriers depends on attempt frequency, activation free energy, and temperature. We computed the rate of reaction for edge and screw dislocation dipoles at various temperatures, friction coefficients, and shear stresses using Molecular Dynamics (MD), Schoeck's entropy formalism and compared with Hans Kramers rate theory. Rates computed dynamically show dependence on Langevin friction, increasing with weaker friction and showing more correlated events. Statistically, using Schoeck's formalism and computing minimum energy path, we found significant entropic effects at high-temperature regions and transition from Arrhenius to non-Arrhenius behavior near the critical resolved shear values in both edge and screw characters.

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