Kink pair production rates and a new velocity rule for discrete dislocation dynamics

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ABSTRACT

Dislocation motion controls the mechanical properties of crystalline materials, such as strength and ductility. Many important phenomena (pile-ups, pattern formation, cross-slip etc.) are easiest to model using discrete dislocations, yet they occur on length- and time-scales inaccessible to atomistic methods. Elasticity-based discrete dislocation dynamics (DDD) simulations [e.g.1,2] have been developed to bridge the mesoscale gap between atomistic and continuum simulations.

DDD simulations require a phenomenological *velocity rule* to specify each dislocation segment's response $\boldsymbol{v}$ to the stress $\boldsymbol{\sigma}$ it experiences. This rule is typically taken to be linear, $\boldsymbol{v} = \boldsymbol{B} \cdot \boldsymbol{\sigma}$ for some mobility tensor $\boldsymbol{B}$. This reflects the fact that for all but the highest strain rates, inertia can be neglected and the motion is overdamped. However, experiments [3] and computer simulations [4] demonstrate that at moderate applied loads, the dislocation response is an extremely nonlinear function of the applied stress, with $\boldsymbol{v} \propto \boldsymbol{\sigma}^{40}$ being reported in [3].

For stresses below the Peierls stress, dislocation motion proceeds via the thermal nucleation of kink pairs. The calculation of the nonlinear kink pair nucleation rate has long been a theoretical challenge. In this work, a stochastic path integral approach is used to derive a simple, general, and exact formula for this rate, and hence the dislocation velocity as a function of applied stress and temperature [5]. The predictions are in excellent agreement with experimental and computational investigations, and unambiguously explain the origin of the observed extreme nonlinearity. A compact analytical expression relating velocity to stress is supplied, in a form suitable for straightforward implementation in DDD simulations.

The theoretical results can also be applied to other systems modelled by an elastic string interacting with a periodic potential, such as Josephson junctions in superconductors.

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