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Phase Field Dislocation Dynamics (PFDD) for Nanoscale Metals

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ABSTRACT

The purpose of this research is to investigate these nanoscale deformation processes through the development and application of a 3D phase field dislocation dynamics (PFDD) model. The phase field approach is centered on energy minimization; hence evolution of the phase field variables has a direct dependence on system energetics. The total system energy is comprised of several contributions that can depend on the problem of interest. Most common are elastic contributions that take into consideration dislocation-dislocation interactions, interactions with an applied stress, and a generalized stacking fault energy term. In particular, the latter term is used to model extended stacking faults and partial dislocations. In this case, the 3D PFDD model can be informed directly by atomistic simulations in order to incorporate a dependence on the entire material gamma-surface as opposed to only one or two stacking fault energies. Additionally, this third energy term can be used to account for the directional motion of dislocations as in body-centered cubic (bcc) metals, where edge dislocations are easier to move than screw dislocations due to differences in the dislocation core structure. Other adjustments have made it possible to address dislocation transmission through interfaces. In this talk, the PFDD approach will be presented and recent results addressing dislocation transmission through interfaces along with other extensions will be discussed.