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Coupling dislocation motion with atomic diffusion

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Abstract

Diffusion has a crucial influence on dislocation motion, particularly at elevated temperatures. It is generally believed that, in a single crystal, lattice diffusion prevails when the temperature is high and core diffusion dominates at relatively low temperatures. Due to the complexity of modelling the coupling between core and lattice diffusion, a given physical problem is often simplified into two extremes where only one of the two diffusion regimes is considered. However, a quantitative definition of the condition under which each of the diffusion mechanisms is dominant is still lacking. In the present work, we employ a variational principle for the analysis of microstructure evolution; we demonstrated how finite element (FE) based analysis can be developed from it, in which the competition and synergy between core diffusion and lattice diffusion can be naturally taken into consideration. A dislocation climb model is further developed by incorporating the FE analysis into the nodal-based three-dimensional dislocation dynamics framework, which also considers glide and cross-slip processes.

Keywords:

dislocation dynamics diffusion climb dislocation plasticity