Coupling Phase-Field Crystal and Field Dislocation Mechanics in Dislocation Modeling

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Abstract

Dislocations are crystalline defects that serve as primary carriers of plastic deformation. Dislocation-based mechanisms are typically modeled via molecular dynamics or discrete dislocation dynamics models; the latter relies on a large set of interaction rules, and both are severely limited in temporal and spatial scales. In this work, we introduce a novel approach to model dislocation dynamics with an atomic resolution and at diffusive time scales by coupling the Phase Field Crystal (PFC) and Field Dislocation Mechanics (FDM) models. PFC had shown great potential in capturing the evolution of topological defects in crystalline materials, but it fails to correctly capture elastic distortions and dynamics. In contrast, FDM captures the latter, but it is unable to keep dislocation cores compact due to its PDE based construct. This work addresses different coupling strategies between PFC and FDM to extract the best of both models. The resulting framework opens pathways for modeling dislocation motion and interactions at diffusive time scales with atomic-level resolution.

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