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Multiscale Crystal Defect Dynamics and Simulation of Fractures

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In this work, we present a novel theory, computation, and validation of a multiscale crystal defect dynamics (MCDD) that is based on an atomistic-informed multiscale process zone (AMPZ) finite element method. We apply it to simulate dislocation motions and fractures in crystalline solids. The main technical ingredients o the multiscale crystal defect dynamics are: (1) Process zone super lattice modeling of crystalline solids and defects; (2) Embedded atom method (EAM)-based constitutive modeling of materials and defects; (3) High order Cauchy-Born rule-based strain gradient formulation for differen order of process zones, and (4) Barycentric finite element technique for polygonal and polyhedral defect finite elements. The proposed multiscale crystal defect dynamics (MCDD) provides an efficient and viable alternative between atomistic molecular dynamics and elastic dislocation dynamics for simulations of defect evolutions such as voids, dislocations, and grain boundaries, twin boundaries, etc. In particular, MCDD provides a mesoscale description on both dynamic lattice microstructure and defect microstructure, and their interactions. The method may provide a multiscale solution for simulation of nanoscale or mesoscale polycrystalline plasticity.

Keywords: Multiscale simulation, crystal defect, dislocation dynamics, fracture,