Multiscale Crystal Defect Dynamics Model and Simulation of Nanoindentation and Dislocation Nucleation

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Abstract

Dislocation nucleation plays a critical role in investigating and understanding the mechanism of plasticity during nanoindentation. In the present study, a multiscale crystal defect dynamics (MCDD) model is developed to simulate the nanoindentation and predict dislocation nucleation. The main novelties of present work are:(1) The dual-lattice tessellation is employed to construct a dual-lattice process zone model which represents various types of defects inside the crystal; (2) A higher order (up to the fourth order) hierarchical strain gradient theory is adopted to model the constitutive relations of various defect process zones, where the atomistic-informed higher order Cauchy-Born rule is used; (3) The finite element bubble mode is added into the lower order element to capture high order strain gradient effects; (4) The contact force of the rigid indenter is derived analytically to reduce the double volume integration to single volume integration, which saves computational efforts greatly. The efficiency of MCDD model allows for simulations at large scales while considering the atomistic interactions. The MCDD model is validated by comparisons with the results of molecular dynamics (MD) for two-dimensional nanoindentation of single crystal copper. Results of three-dimensional nanoindentation have shown that MCDD model can predict dislocation nucleation induced elastic instability automatically and may provide a solution to explore the mechanism of plasticity.

Keywords: Defect mechanics, Dislocation nucleation, Nanoindentation, High-order Cauchy Born rules, Multiscale simulation.