A Multiscale Dislocation Pattern Dynamics: Towards An Atomistic-informed Crystal Plasticity Theory

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Abstract

Dislocations in a deformed crystal tend to aggregate into various dense formations separated by relatively dislocation free regions. These dense formations are called dislocation patterns that underlie most important crystal plasticity features such as work hardening and strain localization. In this work, we put forth a novel concept of the *geometrically compatible dislocation pattern (GCDP)*, and we further show that the previously developed multiscale crystal defect dynamics (MCDD) method (Li et al. (2015) Philosophical Magazine, **94**,1414-1450. and Lyu and Li, (2017) Journal of Mechanics and Physics of Solids, **107**, 379-410.) is actually a discrete dislocation pattern dynamics that can describe evolutions of geometrically compatible dislocation patterns, which may be the dominant dislocation patterns at early stage. The main developments of present work are: (1) We demonstrated that the geometrically compatible dislocation pattern is related to the original crystal lattice microstructure as part of material genome; (2) Using a hierarchical strain gradient formulation, we justified that the multiscale crystal defect dynamics is indeed a multiscale dislocation pattern dynamics, and (3) We showed that the multiscale dislocation pattern dynamics may lead to an atomistic-informed crystal plasticity theory. In doing so, we have developed a MCDD based crystal plasticity finite element method (CPFEM) to simulate crystal slip and shear band formation in single crystals at sub micron scale. The work is highlighted by the use of the MCDD method capturing different types of dislocation patterns, and early cyclic plastic responses of FCC crystals.

Keywords: Crystal plasticity, cyclic plasticity, defect mechanics, dislocation pattern dynamics, high-order Cauchy-Born rules, multiscale simulation.

1. Introduction

One of the longstanding scientific endeavors in computational materials science is to understand, model, and simulate crystal defect evolution and its statistical consequences,

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