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Coarse-grained atomistic simulations of dislocations in Al, Ni and Cu crystals

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ABSTRACT

This paper presents the application of a recently developed concurrent atomistic continuum (CAC) methodology in coarse-grained (CG) atomistic simulations of dislocation nucleation and migration in face-centered cubic (fcc) Al, Ni and Cu crystals, using an EAM force field and an adaptive mesh refinement strategy. The CAC method is based on recently developed atomistic field theory (AFT) that frames the problem in terms of a continuum field representation of lattice and sublattice atomic arrangements. Four sets of CG models with different finite element mesh refinement are constructed to test the accuracy and efficiency of the CG method relative to full molecular dynamics (MD). Simulation results show that the CG method is able to reproduce key phenomena of dislocation dynamics in initially defect free fcc crystals, including strain bursts caused by dislocation nucleation and migration, the structure of leading and trailing partial dislocations separated by equilibrium stacking faults in Al, formation of intrinsic stacking fault ribbons in Ni and Cu, and 3D migration of curved dislocations, all comparable with results of MD simulations. CG simulations have also revealed that the yield strength of Al depends on the thickness of the specimens as well as the operative deformation mechanisms. The effects of mesh size and adaptive mesh refinement on CG simulation results are analyzed and discussed.

1. Introduction

Experimental observations show that dislocations in metals or ceramics exhibit pattern formation or substructuring during plastic deformation, with characteristic length scales of these dislocation structures ranging from hundreds of nanometers to microns (Rudolph, 2005; Landau et al., 2009). While it is clear that resolving dislocation core structures requires full atomic resolution, material interior to dislocation walls in these substructures is nearly dislocation free. Such heterogeneous distribution of defects in dislocation mediated plastic deformation necessitates coarse-grained simulation or multiscale simulation for practical consideration of such phenomena.

Similarly, while dislocation reactions with grain boundaries and interfaces must be atomistically resolved (Spearot et al., 2007; Tschopp and McDowell, 2008; Tucker and McDowell, 2011), the long-range interactions of defects, such as Eshelby dislocations (Weinberger, 2011), in bulk domains can be addressed with coarse-graining strategies to decrease the computational degrees of freedom. Dislocation dynamics (DD) is a popular coarse-graining approach for modeling metal plasticity (Amodeo and Ghoniem, 1990a,b; van der Giessen and Needleman, 1995; Zbib et al., 1998; Groh et al., 2009; Wang and Beyerlein, 2011).

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DD may be considered as a component of a hierarchical multiscale modeling method; for example, Bulatov et al. (1998) used MD simulations to inform local dislocation interaction rules in DD simulations, facilitating simulation of mesoscale dislocation networks with the atomistic detail smeared out. Another hierarchical multiscale approach is to use MD simulations to inform reduced order crystal plasticity descriptions (Zbib and Diaz de la Rubia, 2002; McDowell, 2008).

The aim of the current work is directed more towards concurrent multiscale modeling. Use of disparate models such as quantum mechanics, molecular dynamics, and continuum mechanics within one simulation is a common tactic for addressing problems where full atomistic resolution is required to model certain atomic scale structures and processes while retaining the capability to model long range fields with coarse-grained descriptions. Concurrent multiscale models pursue parallel solutions of the various models in time and space, facilitating the ability to effectively "zoom" in and out of highly refined domains. Two types of concurrent multiscale models have been pursued. The first, otherwise known as coarse-graining, employs multiple models over a common, overlapping spatial domain (e.g., Rudd and Broughton, 1998, 2005; Zhou and McDowell, 2002; Wagner and Liu, 2003; Klein and Zimmerman, 2006; Kulkarni et al., 2008). In this type of coarse-graining approach, the challenge is to transition from atomistic to continuum descriptions without significant simplification, retaining the utility of the underlying interatomic potential, particularly if coarse-scaling of time is attempted as well. The second type of concurrent models employs domain decomposition (Shilkrot et al., 2002a,b; Xiao and Belytschko, 2004) with different models applied in distinct, but overlapping, spatial domains. This approach admits radically different degree-of-freedom descriptions, but is typically limited to the time step of the finest scale model; atomistic simulations are typically employed in some local region of interest such as a crack tip or grain boundary.

As an example of domain decomposition (second type), the Coupled Atomistics Discrete Dislocations (CADD) method (Shilkrot et al., 2002a,b, 2004; Miller et al., 2004; Dewald and Curtin, 2006) was developed to model dislocation plasticity in both atomistic and contiguous continuum regions. In CADD, dislocations may nucleate in the atomistic domain(s) or be introduced from sources within the continuum domain(s). They are then passed through the interface separating the domains in either direction. Discrete dislocation statics or dynamics approaches are employed in the continuum domain. A common issue in such domain decomposition approaches is the attenuation of higher frequency components of lattice vibration at the interface with a continuum region. Moreover, passing curved dislocations with mixed screw-edge character from the atomistic domain across the interface into the continuum (and vice versa) is highly problematic. Another popular domain decomposition approach employs the Cauchy-Born rule-based quasicontinuum (QC) method (Tadmor et al., 1996) in the coarse-grained continuum region. As a lattice statics technique, QC was developed for simulating mechanical responses of crystalline materials through energy minimization. A dynamic version of QC method was developed to simulate dislocation dynamics through adaptive remeshing (Kulkarni et al., 2008). However, in order to accommodate dislocations, the coarse mesh in QC models needs to be adaptively refined down to the atomic scale to capture dislocation nucleation and allow migration. Simulation results show that nearly full atomistic resolution is required in the entire model for simulations involving dislocations.

A new concurrent multiscale approach, the Concurrent Atomistic-Continuum (CAC) method, was recently developed by Chen and co-workers (Chen and Lee, 2005; Chen, 2006, 2009; Deng et al., 2010; Xiong et al., 2009a,b, 2011, 2012). In distinction from existing multiscale methods, the route to coarse-graining is pursued through a multiscale formulation of the dynamics of atomistic systems without the need for domain decomposition. The formulation is an extension of Kirkwood's statistical mechanical theory of transport processes to include subscale internal degrees of a molecule or of a primitive unit cell of crystalline systems. A new set of balance equations is obtained in the form of field representation based on the underlying atomistic information, including the spatial arrangements of atoms in a primitive cell and the interaction between atoms, being naturally built in the formulation. Thus, essential atomistic features are retained in the field representation. As an application of the new formulation, CG simulations have reproduced key phenomena of dislocation dynamics (Xiong et al., 2011). In addition, CAC simulations (Xiong et al., 2012) allow passage of both straight and curved dislocations from the atomistically-resolved region to the coarse-grained finite element region and vice versa, since the same underlying formulation is used in both. In CAC, the interatomic potential is used for all regions, and the degrees of freedom are reduced substantially in CG regions. However, the time step is dictated by that required in the atomistic region, as typical of concurrent methods.

The objective of this paper is to demonstrate the applicability of this new multiscale method in CG simulations of dislocation dynamics in Al, Ni and Cu using reasonably accurate EAM interatomic potentials and an adaptive mesh refinement technique. Following the introduction, finite element implementation of CAC is briefly introduced in Section 2; CG simulations of dislocations in single crystal Al, Ni and Cu under tension are presented in Section 3; major findings are summarized in Section 4. Summary and discussions close the paper in Section 5.

2. Methodology

Kirkwood's statistical mechanical theory of transport processes provides a coarse-grained description of molecular systems using a field representation (Kirkwood, 1946; Irving and Kirkwood, 1950). The formulation started with a field definition of local densities in terms of the positions and momentum of molecular centers in the phase space, and derived the classical transport equations (balance equations) of hydrodynamics as a consequence of Newtonian mechanics. Motivated by Kirkwood's idea of extending his formulation to molecules possessing internal degrees of freedom (Kirkwood, 1946)