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A quasistatic implementation of the concurrent atomistic-continuum method for FCC crystals

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ABSTRACT

In recent years, numerous partitioned-domain methods have been developed to describe dislocation behavior at length scales that are usually inaccessible to most classical atomistic methods. These methods retain full atomistic detail in regions of interest while using a continuum description to reduce the computational burden elsewhere. In most of these methods, however, lattice defects in the continuum are either implemented via constitutive relations, lattice elasticity with dislocation field interactions, or are not permitted at all. In such approaches, the transit of dislocations across the atomistic/continuum interface appeals to approximate heuristics intended to minimize the effects of the interface due to the change from atomistic to continuum degrees of freedom. The concurrent atomistic-continuum (CAC) method, originally developed for addressing dynamic dislocation behavior by Xiong et al. (2011), permits dislocations to propagate in a continuum domain that employs a piecewise continuous finite element description with interelement displacement discontinuities. The method avoids ghost forces at interface between atomistically resolved and coarse-grained domains. CAC has subsequently been used to investigate complex dislocation behavior in face-centered cubic (FCC) metals (Xiong et al., 2012b,a,c, 2015). In this paper, we propose a quasistatic 3-D method to carry out sequential energy-minimized simulations at 0 K. This facilitates study of structure evolution along minimum energy pathways, avoiding over-driven conditions of high rate molecular dynamics. Parallelization steps in code implementation are described. Applications are presented for the quasistatic CAC method in FCC metal plasticity. Comparisons are made with a fully-resolved atomistic method for generalized stacking fault energy, core structure and stress field of a single 60° mixed type dislocation, surface indentation, and 60° mixed type dislocation migration through the interface between atomistic and coarse-grained domains. It is shown that 3-D CAC simulations are useful in substantially reducing the number of degrees of freedom while preserving key characteristics of dislocation structure, stacking faults, and plasticity, including the net Burgers vector and long range fields of interacting dislocations.

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1. Introduction

Metal plasticity is a multiscale phenomenon that is manifested by irreversible microstructure rearrangement associated with nucleation, multiplication, interaction, and migration of dislocations (McDowell, 2010). Long range field interactions between dislocations are extremely important to describe, along with the dissociated character of partial dislocations. The former necessitates large solution scales, while the latter demands treatment of core effects using accurate underlying interatomic potentials. Metal plasticity therefore requires concurrent coupling across various scales. While methods such as molecular dynamics (MD) and discrete dislocation dynamics (DDD) have been widely employed for problems at respective spatial scales involving core effects and long range fields, efforts have been made to concurrently bridge the discrete and continuous descriptions, two fundamentally different approaches (Rudd and Broughton, 2000). Chen et al. (2011) reviewed the theoretical foundations of coarse graining methods and analyzed several representative coarse graining models. A review of 14 concurrent multiscale modeling methods is presented by Miller and Tadmor (2009), and is further summarized by Tadmor and Miller (2012).

Concurrent multiscale methods can be categorized as hierarchical and partitioned-domain methods, where the latter divides the system into atomistic and continuum domains. An example of a partitioned-domain method is the coupled atomistic and discrete dislocation (CADD) method (Shilkrot et al., 2004). The CADD model permits the transfer of dislocations across the interface between the atomistic and continuum domains. It has been employed to incorporate long range fields of dislocation pileups to study the impingement of dislocations on symmetric tilt grain boundaries (GB) in Al by Dewald and Curtin (2007a,b,2011). However, CADD is restricted in that heuristic, *ad hoc* treatments are introduced to pass dislocations through the continuum–atomistic interface; dislocations are detected on one side of the interface and inserted into the other. Moreover, the treatment of curved dislocations of mixed character that might cross domain interfaces is problematic.

Another concurrent atomistic-continuum approach is the quasicontinuum (QC) method (Tadmor et al., 1996). The QC method uses the change of deformation gradient to distinguish domains where full atomistic resolution is required from those where the deformation field varies more smoothly. Representative atoms (repatom) are employed to reduce the degrees of freedom to a small fraction of those required in fully resolved atomistic simulations. The system energy, based on the repatoms, is minimized so that the lattice statics at 0 K is reproduced (Miller and Tadmor, 2002). Recently, the QC method has been extended to include a dynamic, finite temperature formulation (Dupuy et al., 2005; Kulkarni et al., 2008; Tadmor et al., 2013). In such approaches, it is difficult to avoid introduction of a ghost force at the atomistic/continuum interface. Also, since the defects can only nucleate and migrate within the fully atomistic domain, *ad hoc* criteria are needed to assist in adaptive mesh refinement (Shimokawa et al., 2009).

To the authors' knowledge, most partitioned-domain methods, including CADD and QC, treat the continuum domain such that lattice dislocations are either implemented via elastic constitutive relations, or not permitted at all. This motivated development of a new partitioned-domain method called the concurrent atomistic-continuum (CAC) method that employs piecewise continuous first order shape function and interpolation function within elements and admits displacement discontinuities between elements (Xiong et al., 2012a). Boundary layers are employed near element interface to accommodate additional inhomogeneous deformation. In this way, nucleation of dislocations and transport between fully resolved atomistic and coarse-grained domains are permitted, without requiring heuristic rules or overlapping pad regions. Ghost forces are avoided at such interfaces.

The theoretical foundation of the CAC method is the atomistic field theory (AFT). It is rooted in micromorphic theory, where a local density function is used to connect the micromorphic theory and molecular dynamics, in which a crystalline material is viewed as a continuous collection of lattice points, while embedded within each point is a unit cell with a group of discrete atoms (Chen and Lee, 2005). The same balance equations for both fully resolved atomistic and coarse-grained continuum domains are employed to compute the properties of general crystals. In the continuum domain, the interatomic potential serves as the only constitutive relation. The AFT was originally designed with multi-atom crystalline materials in mind (Chen and Lee, 2003a,b), and CAC has been applied on strontium titanate (Yang et al., 2013b; Yang and Chen, 2015) and phonon properties of the 1-D polyatomic crystals (Xiong et al., 2014a).

For monoatomic crystalline materials, each primitive unit cell contains only one atom. Xiong et al. (2011) performed CAC simulations to reproduce the complex dislocation phenomena in FCC metals such as dislocation nucleation/migration and formation of multiple stacking fault ribbons. Deng et al. (2010) and Deng and Chen (2013) studied the wave and crack propagation, as well as the impact fracture in an ideal brittle material. More recently, the embedded atom method (EAM) potential was incorporated in CAC simulations to study more general dislocation behavior such as migration of curved dislocations, formation of leading and trailing partial dislocations, dislocation loop coalescence, dislocation–phonon interactions, and dislocation–void interactions in pure FCC crystals (Xiong et al., 2012b,c,a, 2014b, 2015).

The objective of the present work is to briefly review the basic formulations in AFT, formulate a new quasistatic 3-D CAC method that employs sequential energy minimization for problems involving dislocation migration and interaction with domain interface, detail the numerical implementation, and demonstrate its applicability to metal plasticity involving arrays of dislocations in pure FCC crystals. Since the quasistatic CAC method facilitates exploration of structure evolution along minimum energy pathways, in contrast to over-driven MD simulations at high rates, we explore how the quasistatic CAC method provides largely satisfactory predictive results for benchmark simulations at a much lower computational cost than