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Concurrent atomistic–continuum simulations of dislocation–void interactions in fcc crystals

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ABSTRACT

Dislocation interactions with distributed condensed vacancy clusters in fcc metals were simulated via a concurrent atomistic–continuum method. Due to void strengthening, the dislocation lines are found to bow as a result of pinning on the original glide plane and undergo depinning through drawing out screw dipoles and forming prismatic loops on the secondary slip plane. We discovered an inertia-induced transition between Hirsch looping and void shearing mechanisms as the void spacing ranges from the scale of nm to hundreds of nm. Contrary to prior understanding, simulations suggest that large voids (~5 nm in diameter) can behave as weak barriers to dislocation motions under high strain-rate dynamic conditions.

1. Introduction

Materials subjected to irradiation exhibit elevated yield strength and suffer from intrinsic softening and reduced ductility by virtue of localization of dislocation plasticity. Irradiation-induced defects act as obstacles to dislocation migration. Typical radiation-induced defects in fcc lattices include voids (Averback et al., 1977; Kluth et al., 2005; Kondo et al., 2008, Crocombette and Proville, 2011) and helium bubbles (Donnelly et al., 1983; Henriksson et al., 2005; Demkowicz et al., 2010; David et al., 2011), particularly for fusion applications (Zinkle, 2005). Transmission electron microscopy (TEM) studies indicate that these defects act as obstacles to dislocations and, when bypassed, lead to localization of deformation in regions where defect densities are reduced via dislocation interaction (Shilo and Zolotoabko, 2003, 2007; Shingo et al., 2007; Wu et al., 2007). Unfortunately, in situ observations of dislocation–obstacle interactions are quite limited owing to elaborate sample preparation, and restricted spatial and temporal ranges of TEM.

Static analysis of void strengthening suggests that voids with diameter of ~2 nm or larger generally act as 'strong obstacles', whereas voids with diameter less than ~2 nm act as 'weak obstacles', respectively (Hull and Bacon, 2001). It was concluded that the stress required for dislocation depinning from these voids approaches the theoretical Orowan stress (Hull and Bacon, 2001; Hirth and Lothe, 1982; Shim et al., 2007). For predicting the in-service performance of metals in fusion energy facilities, however, understanding of the influence of dynamic deformation on void strengthening mechanisms is crucial and requires atomistic insight of unit processes of dislocation–void interactions. In the past ten years, molecular dynamics (MD) has been used extensively to investigate dislocation–obstacle interactions in irradiated metals (Wu et al., 2007; Shim et al., 2007; Harry and Bacon, 2002; Osetsky and Bacon, 2003; Bacon and Osetsky, 2005; Bacon et al., 2006;

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Terentyev et al., 2007; Cheng et al., 2010). Major limitations arise in using MD to simulate large systems, for example systems with dislocation line lengths on the order of microns and void spacing on the order of hundreds of nanometers. Continuum simulation tools such as dislocation dynamics (DD) (Amodeo and Ghoniem, 1990a, 1990b; Kubin and Canova, 1992; Van der Giessen and Needleman, 1995; Zbib et al., 1998; Bulatov et al., 1998; Cai and Bulatov, 2004) provide approximate description of dislocations at these larger scales, based on elastic theory of lattice dislocations. However, DD typically suffers from the approximate nature of prescribed short-range interaction rules between mobile dislocations and obstacles, lacks the ability to model dislocation dissociation, and requires approximations for dislocation cross slip and other important local mechanisms.

Pioneering MD simulations of vibrating dislocations were conducted but limited to 2D Frenkel–Kontorowa models (Weiner et al., 1976). Those models neglected phonon drag effects. Recently, Gumbsch and co-workers (Cheng et al., 2010, Bitzek and Gumbsch, 2004, 2005) investigated dislocation depinning through MD simulations considering dynamic/inertial effects. Their results suggest that dynamic inertial effects significantly lower the depinning stress. It was suggested that such inertial effects should not be ignored in computational models at higher scales. However, continuum models, such as DD, typically assume overdamped dislocation migration via a constitutive force–velocity relationship.

Due to the spatio-temporal complexity of dislocation dynamics, various multiscale modeling methods (McDowell, 2010) including sequential (Amodeo and Ghoniem, 1990a, 1990b; Kubin and Canova, 1992; Van der Giessen and Needleman, 1995; Zbib et al., 1998; Bulatov et al., 1998; Cai and Bulatov, 2004; Shehadeh et al., 2006; Hu et al., 2007) and concurrent (Tadmor et al., 1996; Zhou and McDowell, 2002; Fago et al., 2004; Shilkrot et al., 2002a, 2002b; Zamora et al., 2012) approaches have been developed to describe dislocation physics. In sequential, hierarchical multiscale modeling approaches, it is intended that the characteristics and understanding of dislocation–obstacle interactions obtained from MD are incorporated in higher length scale continuum DD or crystal plasticity simulations. These parameters include maximum obstacle force, critical cusp angle, and Peierls stress. Although particular long range dislocation–obstacle interactions can be represented within continuum treatments, it is difficult if not impossible to address complex short range interactions and processes (e.g., core interactions). Concurrent approaches such as the Quaiscontinuum method (QC) (Tadmor et al., 1996; Fago et al., 2004) or Coupled Atomistics Discrete Dislocation (CADD) (Shilkrot et al., 2002a, 2002bb; Zamora et al., 2012) seek to address the crucial question of how to reconcile a consistent treatment of dislocations that pass between atomic and continuum regions; heuristic numerical techniques and/or rules are invoked for passing dislocations across interfaces between atomistic and continuum domains or through coarse-grained continuum domains with adaptive mesh refinement. As a consequence of these specialized treatments, existing concurrent approaches are only suitable for 2D quasistatic simulations of dislocations. For 3D dynamic dislocation–obstacle interactions, the recently developed concurrent atomistic–continuum (CAC) method (Xiong et al., 2011, 2012a, 2012b) is suitable as a formal coarse-graining of MD and is pursued in this work.

2. Methodology

Fundamental to the CAC method is a unified formulation of atomistic and continuum representation of balance laws (Chen and Lee, 2005; Chen, 2006, 2009). The CAC formulation generalizes Kirkwood's statistical mechanical theory of transport processes (Kirkwood, 1946; Irving and Kirkwood, 1950) to facilitate a two-level structural description of materials. It describes the structure of a crystalline material in terms of continuously-distributed lattice cells, but with a group of discrete atoms situated in each lattice cell at sub-structural level. A complete field representation of balance laws of atomistic systems is then derived. Under elastic distortion, the new balance equations fully reproduce the phonon dispersion relations (Xiong et al., 2014b). Consequently, the formulation reflects all possible dynamics on length and time scales from the atomic to the macroscopic, and admits coarse-graining in the context of a finite element formulation in which large numbers of atoms are contained within each element, with defects (e.g., dislocations or cracks) propagating along discontinuous element interfaces. This avoids anomalous effects of atomistic–continuum interfaces that hamper domain decomposition methods such as CADD (Shilkrot et al., 2002a, 2002b; Zamora et al., 2012), as well as finite temperature extensions of adaptively remeshed or reconfigured QC methods (Kulkarni et al., 2008). In contrast to most existing multiscale or coarse-grained methods (Chen et al., 2011), the representation of the complete set of balance laws renders CAC applicable to dynamic and nonequilibrium processes involving mass, momentum, and/or energy transport (Xiong et al., 2014b), with the interatomic potential or force field being the only empirical input. This work employs the embedded atom method potential (Daw and Baskes, 1984) for Ni (Mishin et al., 1999, 2001). The numerical implementation code of CAC is parallelized and is run on $N = 72$ processors, scaling as $O(N)$. The present work considers balance of mass and momentum, without addressing the energy equation, in view of the focus on dynamic effects of dislocation–void interactions.

3. Computational set-up and results

3.1. Effects of void spacings on the dislocation pinning–depinning

Fig. 1 shows the computational configuration of CAC models in this study. Single crystal Ni specimens ($\sim 50 \times 200 \times 100\ \text{nm}^3$) contain over 20 million atoms. The V-notch and four spherical voids with diameters of $\sim$5 nm are initially introduced into the models. The distance between the V-notch tip and the centers of the voids is $\sim$40 nm. Here