This paper presents a new methodology for coarse-grained atomistic simulation of dislocation dynamics. The methodology combines an atomistic formulation of balance equations and a modified finite element method employing rhombohedral-shaped 3D solid elements suitable for fcc crystals. With significantly less degrees of freedom than that of a fully atomistic model and without additional constitutive rules to govern dislocation activities, this new coarse-graining (CG) method is shown to be able to reproduce key phenomena of dislocation dynamics for fcc crystals, including dislocation nucleation and migration, formation of stacking faults and Lomer–Cottrell locks, and splitting of stacking faults, all comparable with fully resolved molecular dynamics simulations. Using a uniform coarse mesh, the CG method is then applied to simulate an initially dislocation-free submicron-sized thin Cu sheet. The results show that the CG simulation has captured the nucleation and migration of large number of dislocations, formation of multiple stacking fault ribbons, and the occurrence of complex dislocation phenomena such as dislocation annihilation, cutting, and passing through the stacking faults. The distinctions of this method from existing coarse-graining or multiscale methods and its potential applications and limitations are also discussed.

© 2010 Elsevier Ltd. All rights reserved.

1. Introduction

Plastic deformation of ductile metals involves multiple length and time scales ranging from dislocation nucleation at the atomic scale to the formation of multiple slip bands, planar dislocation arrays, and dislocation cells at submicron and micron scales, to the observable effect of plastic deformation at the macroscopic scale. It has been argued that such multiscale material behavior precludes direct calculation using a formulation appropriate for the governing scale (Wallin et al., 2008). Accordingly, many multiscale methods for modeling plasticity have been developed in the past 10 years. Existing popular multiscale methods may be divided into two categories: sequential and concurrent multiscale methods.

Sequential or hierarchical methods address a range of length scales by passing parameters or descriptions from small-scale calculations to larger scale models. Physical phenomena are modeled at different scales and material responses at small scales are used to inform large-scale models with reduced degrees-of-freedom. For plasticity modeling, these methods usually require a sophisticated understanding of the physics of dislocation dynamics based on atomistic simulations to develop constitutive laws to model dislocation nucleation, the strength of dislocation junctions, dislocation mobility, dislocation interactions, etc. in large-scale continuum simulations (Amodeo and Ghoniem, 1990a; b; van der Giessen and...
Needleman, 1995; Zbib et al., 1998; Groh et al., 2009). At still higher scales, hierarchical models are used to inform reduced order crystal plasticity descriptions (Bulatov et al., 1998; Zbib and Díaz de la Rubia, 2002; McDowell, 2008).

In contrast, concurrent multiscale modeling methods address multiple length and time scales by coupling different methods in a single analysis (Broughton et al., 1999; Cai et al., 2000; Zhou and McDowell, 2002; Wagner and Liu, 2003; Xiao and Belytschko, 2004; Klein and Zimmerman, 2006). Examples of successful concurrent methods for modeling dislocation plasticity that employ domain decomposition include the coupled atomistic and discrete dislocation (CADD) formulation (Shilkrot et al., 2002a, b, 2004; Miller et al., 2004; Dewald and Curtin, 2006) and coupled discrete dislocation and continuum crystal plasticity (Wallin et al., 2008). A crucial component of these domain decomposition methods is achieving physical congruence across the interface between different theoretical descriptions of the same material. For multiscale modeling of quasistatic plasticity, passing dislocations from a domain with discrete description across the interface to the continuum description has been a significant issue for three-dimensional (curved) dislocation lines. For dynamic multiscale modeling of plasticity, wave reflections at the interface arising from the lower frequency and large wavelength limits of the continuum domain may fundamentally alter the material behavior, introducing unphysical phenomena into the simulation. Various damping approximations have been introduced to alleviate this problem, largely of ad hoc character.

The quasicontinuum method is a mixed continuum and atomistic approach developed by Tadmor et al. (1996) for simulating the mechanical response of crystalline materials at zero temperature. The method is based on energy-minimization and aims to reproduce the results of standard lattice statics at a fraction of the computational cost (Miller and Tadmor, 2008, 2009). Recently, this method has been extended to treat systems with finite temperature by replacing the conventional position-dependent interatomic potentials with position-temperature-dependent ones, and treating time-dependent phenomena as a sequence of incremental problems (Kulkarni et al., 2008). This method was demonstrated through simulations of a nanoindentation test with adaptive remeshing. In their mixed coarse-grained and atomic simulations, dislocation nucleation was observed, but the stacking faults were unable to pass from the atomistic to the coarse-grained region. Moreover, with a higher mesh refinement tolerance, almost fully atomistic resolution was required to model dislocation nucleation.

The objective of this paper is to present a new and different coarse-grained methodology for dynamic simulation of dislocations and plasticity and to test its accuracy and efficiency relative to MD. The methodology combines (1) a continuum field representation of balance equations for metallic crystals with fully atomistic information built into the formulation and (2) a modified finite element method employing rhombohedral-shaped 3D linear solid elements. The theoretical formulation follows the formalism developed by Kirkwood (1946), Irving and Kirkwood (1950), and Hardy (1982), a successful statistical mechanics procedure in linking the atomistic model to the local properties and balance equations in classical continuum representation. Similar work following this formalism can be found in Chen and Lee (2003a, b), Delph (2005), Chen (2006), Zimmerman et al. (2004), Webb et al. (2008), and Zimmerman et al. (2010). A different formulation that is a further generalization of the Kirkwood–Hardy formalism for materials with general lattice structure (materials that have more than one atom in the primitive unit cell) can be found in Chen and Lee (2005) and Chen (2009). The present formulation is useful for modeling point and line defects in crystalline solids. It can be viewed as a special case of the general formulation, obtained as an exact consequence of Newton’s second law following classical statistical mechanics.

Following the introduction, the continuum representation of balance equations is formulated from atomistic N-body dynamics and presented in a mathematical form that facilitates the simulation of discontinuities in Section 2; finite element implementation of the formulation is introduced in Section 3; numerical examples of coarse-grained atomistic simulation of single-crystal copper are shown in Section 4. The fundamental difference between the present methodology and existing coarse-graining methods or multiscale methods is summarized in Section 5, where limitations of the present coarse-graining method are also discussed.

2. Atomic formulation of microscopic balance equations

Continuum description of physical quantities is by means of continuous functions of the spatial coordinates \( \mathbf{x} \) and time \( t \). Microscopic dynamic quantities in classical N-body dynamics, on the other hand, are functions of phase-space coordinates \( (\mathbf{r}, \mathbf{p}) \), i.e., the positions and momenta of atoms:

\[
\mathbf{r} = (\mathbf{R}^k, k = 1, 2, 3, \ldots, n), \\
\mathbf{p} = (m^k \mathbf{V}^k, k = 1, 2, 3, \ldots, n).
\] (2.1)

Here, \( \mathbf{R}^k \) is the position vector and \( \mathbf{V}^k \) is the velocity vector of the \( k \)-th atom, \( m^k \) is the atomic mass, and \( n \) is the total number of atoms in the system. Following the instantaneous microscopic representation (Hardy, 1982; Evens and Morriss, 1990), rather than the ensemble-based Irvine–Kirkwood formulation (1951), the link between a phase space dynamic function \( \mathbf{A}(\mathbf{r}, \mathbf{p}) \) and the corresponding local density function \( \mathbf{a}(\mathbf{x}, t) \) in physical space can be defined as

\[
\mathbf{a}(\mathbf{x}, t) = \sum_{k=1}^{n} A(r(t), p(t)) \delta(\mathbf{R}^k(t) - \mathbf{x}).
\] (2.2)

Here, the localization function, \( \delta(\mathbf{R}^k - \mathbf{x}) \), has units of inverse volume. It can be a Dirac \( \delta \)-function (Irving and Kirkwood, 1950) or a distribution or weighting function (Hardy, 1982). The time dependence of the densities is contained in the time dependence of the positions and velocities of the individual particles (Hardy, 1982; Chen, 2006).
In classical statistical mechanics, density functions of the form in Eq. (2.2) are called localized quantities or microscopic local densities, and the macroscopic local densities, \( \bar{\rho}(\bf{x},t) \), are defined as averages of the microscopic density functions via ensemble averaging. The general form is

\[
\bar{\rho}(\bf{x},t) = \int \int \int \sum_{k=1}^{n} m_k \delta(\bf{R}^k - \bf{x}) f(\bf{r},\bf{p},t) \, d\bf{r} \, d\bf{p},
\]

where \( f(\bf{r},\bf{p},t) \) is the distribution function. Eqs. (2.2) and (2.3) distinguish microscopic field quantities from ensemble-averaged macroscopic field quantities.

From Eq. (2.2), the microscopic local mass density \( \rho \) (mass per unit volume), momentum density \( \rho \bf{v} \), and total energy density \( \rho e \) (energy per unit mass) can be defined as (Hardy, 1982; Chen, 2006)

\[
\rho(\bf{x}) = \sum_{k=1}^{n} m_k \delta(\bf{R}^k - \bf{x}),
\]

\[
\rho(\bf{x})\bf{v}(\bf{x}) = \sum_{k=1}^{n} m_k \bf{v}^k \delta(\bf{R}^k - \bf{x}),
\]

\[
\rho(\bf{x})e(\bf{x}) = \sum_{k=1}^{n} \left[ \frac{1}{2} m_k (\bf{v}^k)^2 + U^k \right] \delta(\bf{R}^k - \bf{x}),
\]

where \( U^k \) is the potential energy, \( \frac{1}{2} m_k (\bf{v}^k)^2 + U^k = E^k \) is the atomic site energy of the kth atom, and \( \bf{v} \) is the velocity field with \( \bf{v} = \rho \bf{v} / \rho \). With Newton’s second law and the identity

\[
\nabla_x \delta(\bf{R}^k - \bf{x}) = -\nabla_x \delta(\bf{R}^k - \bf{x}),
\]

the time derivatives of Eqs. (2.4)–(2.6) are found to be

\[
\frac{d\rho}{dt} = -\nabla_x \cdot \sum_{k=1}^{n} m_k \bf{v}^k \delta(\bf{R}^k - \bf{x}),
\]

\[
\frac{d(\rho \bf{v})}{dt} = \sum_{k=1}^{n} (\bf{F}^k \cdot \bf{v}^k + \bf{U}^k) \delta(\bf{R}^k - \bf{x}) + \bf{f}_{ext} \cdot \nabla_x \times \nabla_x \cdot \nabla_x \bf{v} + \sum_{k=1}^{n} \bf{v}^k \delta(\bf{R}^k - \bf{x}) + \rho e \bf{v},
\]

\[
\frac{d(\rho e)}{dt} = \sum_{k=1}^{n} (\bf{F}^k \cdot \bf{v}^k + \bf{U}^k) \delta(\bf{R}^k - \bf{x}) + \bf{f}_{ext} \cdot \nabla_x \times \nabla_x \bf{v} + \sum_{k=1}^{n} \bf{v}^k \delta(\bf{R}^k - \bf{x}) + \rho e \bf{v}.
\]

Here, \( \bf{f}_{ext}(\bf{x}) \) is the external force field, \( \bf{F}^k \) is the total interatomic force acting on kth atom, \( \bf{V}^k = \bf{v}^k - \bf{v}(\bf{x}) \) is the difference between the phase space particle velocity and the local velocity field. The momentum flux density (the atomic counterpart of stress) is generally defined by \( \bf{t}(\bf{x}) = \bf{t}_{kin}(\bf{x}) + \bf{t}_{pot}(\bf{x}) \) with \( \bf{t}_{kin} \) and \( \bf{t}_{pot} \) given by

\[
\bf{t}_{kin}(\bf{x}) = -\sum_{k=1}^{n} m_k \bf{v}^k \otimes \bf{v}^k \delta(\bf{R}^k - \bf{x}),
\]

\[
\nabla_x \cdot \bf{t}_{pot}(\bf{x}) = \bf{f}_{int}(\bf{x}) = \sum_{k=1}^{n} \bf{F}^k \delta(\bf{R}^k - \bf{x}),
\]

where \( \bf{f}_{int}(\bf{x}) \) is the internal force density; the symbol “\( \otimes \)” represents a tensor product; \( \bf{t}_{kin} \) and \( \bf{t}_{pot} \) are referred as kinetic and potential stresses, respectively, and \( \bf{t}_{pot} \) follows the classical definition of macroscopic stress (Sommerfeld, 1950; Nye, 1957) as “any tensor field that satisfies the condition that its divergence is the vector force field”. Similarly, the conductive flow of internal energy (the heat flux) is defined by \( \bf{q}(\bf{x}) = \bf{q}_{kin}(\bf{x}) + \bf{q}_{pot}(\bf{x}) \) with \( \bf{q}_{kin} \) and \( \bf{q}_{pot} \) being given by

\[
\bf{q}_{kin}(\bf{x}) = -\sum_{k=1}^{n} \bf{v}^k \left[ \frac{1}{2} m_k (\bf{v}^k)^2 + U^k \right] \delta(\bf{R}^k - \bf{x}),
\]

\[
\nabla_x \cdot (\bf{q}_{pot} + \bf{t}_{pot} \cdot \bf{v}) = \sum_{k=1}^{n} (\bf{F}^k \cdot \bf{v}^k + \bf{U}^k) \delta(\bf{R}^k - \bf{x}).
\]

Substituting the definitions of linear momentum, momentum flux, and heat flux into Eqs. (2.8)–(2.10), we obtain

\[
\frac{d\rho}{dt} + \nabla_x \cdot (\rho \bf{v}) = 0,
\]

\[
\frac{d(\rho \bf{v})}{dt} = \nabla_x \times (\bf{t} - \rho \bf{v} \otimes \bf{v}) + \bf{f}_{ext},
\]
\[
\frac{\partial (\rho \mathbf{v})}{\partial t} = \nabla \cdot (\mathbf{q} + \mathbf{t} \cdot \mathbf{v} - \rho \mathbf{v}) + \mathbf{f}_{\text{ext}} \cdot \mathbf{v}.
\]

(2.17)

For systems with pair interaction forces, Irving and Kirkwood (1950), Hardy (1982), and Chen and Lee (2003a, b) have obtained the formulae for stress and heat flux. For general three-body interaction forces, Chen (2006) has obtained the internal force density as

\[
f_{\text{int}}(\mathbf{x}) = -\frac{1}{2} \int_{\mathbf{x}}^{1} \sum_{i=j}^{n} \mathbf{R}_i^j \otimes \mathbf{F} \delta(\mathbf{R}_i^j (1-\lambda) - \mathbf{x}) d\lambda.
\]

(2.18)

and the stress and heat flux as

\[
t(\mathbf{x}) = -\sum_{i=1}^{n} m_i \mathbf{V}_i \otimes \mathbf{V}_i \delta(\mathbf{R}_i - \mathbf{x}) - \frac{1}{2} \int_{\mathbf{x}}^{1} \sum_{i<j}^{n} \mathbf{R}_i^j \otimes \mathbf{F} \delta(\mathbf{R}_i^j (1-\lambda) - \mathbf{x}) d\lambda.
\]

(2.19)

\[
q(\mathbf{x}) = -\sum_{i=1}^{n} \mathbf{V}_i \left[ \frac{1}{2} m_i (\mathbf{V}_i^2 + U_i) \right] \delta(\mathbf{R}_i - \mathbf{x}) - \frac{1}{2} \int_{\mathbf{x}}^{1} \sum_{i<j}^{n} \mathbf{R}_i^j \otimes \mathbf{F}_i^j \delta(\mathbf{R}_i^j (1-\lambda) - \mathbf{x}) d\lambda.
\]

(2.20)

where \( \int_{\mathbf{x}}^{1} \delta(\mathbf{R}_i^j (1-\lambda) - \mathbf{x}) d\lambda \) represents a line segment that links \( \mathbf{R}_i^k \) and \( \mathbf{R}_i^j \) and passes through \( \mathbf{x} \), \( \mathbf{R}_i^j = \mathbf{R}_i - \mathbf{R}_j \), \( \mathbf{F}_i^j = -\partial U_i^j / \partial \mathbf{R}_i^j \) for pair interactions while \( \mathbf{F}_i^j = -\sum_{k \neq i,j} \partial (U_i^j + U_i^k) / \partial \mathbf{R}_i^j \) for three-body interactions, and the many-body potential function, including the Tersoff (1986) and the Stillinger-Weber (1985) potential functions, is expressed in a general form (Chen, 2006) as

\[
U = \frac{1}{2} \sum_{i,j} U_{ij}, \quad U_{ij} = \sum_{k \neq i,j} \left( U_{ij} + U_{ik} + U_{jk} \right).
\]

(2.21)

An instantaneous expression for the temperature in classical many-body dynamics is expressed in terms of the mean-squared velocity relative to the local velocity field (Hoover, 1986, 1991)

\[
T(\mathbf{x}) = \frac{1}{3 \rho_N k_B} \sum_{k=1}^{n} m_k (\mathbf{V}_k^2 - \mathbf{v}^2) \delta(\mathbf{R}_k - \mathbf{x}) = \frac{1}{3 \rho_N k_B} \sum_{k=1}^{n} m_k (\mathbf{V}_k^2 - \mathbf{v}^2) \delta(\mathbf{R}_k - \mathbf{x}),
\]

(2.22)

where \( \rho_N = \sum_{k=1}^{n} \delta(\mathbf{R}_k - \mathbf{x}) \) is the number density (number of atoms per volume), \( k_B \) is the Boltzmann constant, and the kinetic temperature defined in Eq. (2.22) is a measure of the velocity fluctuation (Evans and Morriss, 1990). Eq. (2.9) now becomes

\[
\frac{\partial \mathbf{v}}{\partial t} + \nabla \cdot (\mathbf{v} \otimes \mathbf{v}) + \gamma \nabla T = \mathbf{f}_{\text{int}} + \mathbf{f}_{\text{ext}},
\]

(2.23)

where \( \gamma = 3 k_B \rho_N \). In deriving Eq. (2.23) we have assumed that the kinetic temperature (velocity fluctuation) is isotropic at thermal equilibrium, and hence

\[
t_{\text{int}}(\mathbf{x}) = -\gamma T(\mathbf{x})
\]

(2.24)

3. Numerical implementation by finite element method

Eqs. (2.15)–(2.17) are the microscopic balance equations expressed in terms of local densities and are identical in form to the balance equations of classical continuum mechanics. Thus, continuum modeling techniques such as the finite difference, finite element or meshless methods can be used to solve for the displacement field, and different meshes can be used in various regions of interest. Coarser meshes can be used in regions where the material deforms cooperatively or where local densities do not change rapidly in space; if needed, a coarse mesh can be refined to the atomic scale during simulation to resolve important atomic scale phenomena. In other words, the discretized governing equations at the atomic scale are identical with the governing equations in the atomistic N-body dynamics. Using the concept of shape functions, on the other hand, atomic displacements can be constrained to reduce the majority of degrees-of-freedom in coarse-scale finite element simulations.

Eq. (2.23) is an alternative form of the balance equation of linear momentum. Together with the conservation equation of mass or the definition of mass density and a specified internal force field, they completely govern the material behavior in space and time for systems with a specified temperature, and should reproduce the results of constant-temperature molecular dynamics simulations that employ a thermostat. In such a case, we have

\[
\rho \mathbf{u}(\mathbf{x}) + \gamma \nabla T(\mathbf{x}) = \mathbf{f}_{\text{int}}(\mathbf{x}) + \mathbf{f}_{\text{ext}}(\mathbf{x}),
\]

(3.1)

where \( \mathbf{u}(\mathbf{x}) \) is the displacement field, and generally

\[
f_{\text{int}}(\mathbf{x}) = \int_{\Omega(\mathbf{x})} f(\mathbf{u}(\mathbf{x}), \mathbf{u}(\mathbf{x}')) d\mathbf{x}
\]

(3.2)
is a nonlocal and nonlinear function of relative displacement and can be obtained through fitting to experimental measurements and/or first principles calculations. In this work, the Lennard–Jones (LJ) potential (Kluge et al., 1990) is used to determine the internal force density, with parameters $\sigma_0=0.167$ eV and $\sigma_\sigma=2.3151$ Å that leads to the lattice constant ($a_0$) value of 3.616 Å in the case of Cu. This LJ model potential has a smooth cut off between the fourth- and fifth neighbors at 1.49$a_0$. Because the stable stacking fault energy of FCC lattice via the LJ potential is low, the equilibrium width of the stacking-fault ribbons between the two partials is 9.6$a_0$ (Kogure et al., 1987), whereas the width in the actual Cu crystals is 5$a_0$ (Hull and Bacon, 2001; Mishin et al., 2001). Although the LJ potential is considered to be unsuitable for describing dislocation core structures in FCC metals, it has been shown that the resulting defect configurations modeled by fully atomistic simulations have rather similar appearances to those obtained using the more accurate EAM potential (Kimizuka et al., 2003).

Here, to demonstrate the present method, we employ the simple LJ model. There is no conceptual difficulty in employing the EAM potential.

To seek a coarse-grained description of the atomistic system, we consider a finite element (FE) that contains a collection of material points (i.e., primitive unit cells). We approximate the displacement within this element by

$$\hat{\mathbf{u}}(\mathbf{x}) = \Phi_\mathbf{e}(\mathbf{x}) \mathbf{U}_\mathbf{e} \quad \text{or} \quad \hat{\mathbf{u}}(\mathbf{x}) = \Phi_\mathbf{e}(\mathbf{x}) \mathbf{U}_\mathbf{e}, \quad i = 1,2,3, \quad \zeta = 1,2,..n,$$

where $\mathbf{U}_\mathbf{e}$ are FE nodal displacements, $\Phi_\mathbf{e}(\mathbf{x})$ is the standard FE shape function, $n$ is the number of all unknown parameters in the approximation function ($n=8$ for a linear 8-node 3D solid element), and $\hat{\mathbf{u}}(\mathbf{x})$ represents the interpolated displacement field within the element. The weak form of Eq. (3.1) can be obtained by the Galerkin method (Belytschko et al., 2000) as

$$\int_{\Omega_\mathbf{e}} \Phi_\zeta(\mathbf{x}) \left( \rho \frac{\partial \mathbf{U}_\zeta}{\partial t} + \gamma \nabla_x T(\mathbf{x}) - \int_{\Omega_\mathbf{e}} \mathbf{f}_{\text{int}}(\Phi_\zeta(\mathbf{x}) U_{\zeta}, \Phi_{\mathbf{e}}(\mathbf{x})U_{\mathbf{e}}) d\Omega(\mathbf{x}) - \mathbf{f}_{\text{ext}}(\mathbf{x}) \right) d\Omega(\mathbf{x}) = 0.$$  

(3.4)

The matrix form of Eq. (3.4) can be written as

$$\mathbf{M} \dot{\mathbf{U}} = \mathbf{F}_{\text{int}}(\mathbf{U}) + \mathbf{F}_{\text{ext}},$$

(3.5)

where

$$\mathbf{M} = \int_{\Omega_\mathbf{e}} \rho \Phi_\zeta(\mathbf{x}) \Phi_\zeta(\mathbf{x}) d\mathbf{x},$$

(3.6)

$$\mathbf{F}_{\text{int}}(\mathbf{U}) = \int_{\Omega_\mathbf{e}} \int_{\Omega_\mathbf{e}} \Phi_\zeta(\mathbf{x}) \mathbf{f}_{\text{int}}(\Phi_\zeta(\mathbf{x}) U_{\zeta}, \Phi_{\mathbf{e}}(\mathbf{x})U_{\mathbf{e}}) d\mathbf{x} d\mathbf{x},$$

(3.7)

$$\mathbf{F}_{\text{ext}} = \int_{\Omega_\mathbf{e}} \Phi_\zeta(\mathbf{x}) (-\gamma \nabla_x T(\mathbf{x}) + \mathbf{f}_{\text{ext}}(\mathbf{x})) d\Omega(\mathbf{x}).$$

(3.8)

Eqs. (3.6)–(3.8) can be computed through numerical integration methods such as Gauss integration or nodal integration. In this work, Gauss integration is implemented to calculate the integrals, and the explicit time integration algorithm of the central difference method is used to solve the governing equations with a time step of 5 fs. Since the only constitutive law is the nonlocal internal force–displacement relation and no spatial derivatives are involved in the governing equations for systems with a homogeneous temperature field, connectivity between neighboring elements is not required. Also, the simulation results can be displayed in terms of the FE mesh or in terms of atoms by backmapping the atomic positions from the FE nodal displacements using the interpolation functions.

For the purpose of comparing the CG simulation results with those of MD, the general-purpose parallel MD simulation code DL-POLY (Smith and Forrester, 2001) with the Hoover constant temperature ensemble (NVT) (Hoover, 1985) is employed for the MD simulations. In this work, we concentrate on mechanical aspects of dislocation nucleation and migration; hence, the temperature is set at $T=0.2$ K in all MD and CG simulations presented in this paper. To simulate finite-sized copper thin sheets under tensile loading by both CG and MD, a constant velocity of 5 m/s is applied (corresponding to a strain rate on the order of $10^3$ s$^{-1}$) on the two horizontal ends of each specimen with all of the other surfaces traction free.

4. Simulation results and discussions

To compare the accuracy and efficiency of the CG method relative to MD in modeling dislocation activities, this section presents 6 CG simulations and 6 corresponding MD simulations of initially dislocation-free notched single crystal specimens and 1 submicron-sized CG simulation.

4.1. Dislocation nucleation and migration

Fig. 1 shows the computational set-up for each of three CG models designed to investigate dislocation nucleation and migration as well as the effect of mesh size of the CG method. Table 1 summarizes physical dimensions of the specimens and the different FE mesh sizes employed in the CG simulations. Each model has nearly the same width/length ratio but different thicknesses. All the 3 specimens are discretized into 638 elements with element surfaces along [1 1 1] close-packed planes, as
shown in Fig. 1c. The rhombohedral shape of the finite elements is adopted to mimic the shape of the primitive unit cell of single crystal copper. The rhombohedral-shaped element ensures that, following nucleation, dislocations can glide between elements on either of two (111) or (111) slip systems along element boundaries, in spite of the limitation that the displacement field within each finite element is interpolated from nodal displacement using linear interpolation functions. As shown in Table 1, there are 125 atoms in each finite element in the CG Model-1, 729 atoms in CG Model-2, and 1331 atoms in CG Model-3, corresponding respectively to 6%, 1%, 0.6% of the degrees-of-freedom of the corresponding fully atomistic model.

The stress–strain curves for each specimen simulated using both the CG method and MD are compared in Figs. 2–4. The points at which the first dislocation nucleates are marked as “Nucleation” in each of the Figures. The values of these threshold stress/strain values are also summarized in Table 2. Prior to dislocation nucleation, stress–strain behavior in both CG and MD simulations overlay for all three sets of simulations. While the threshold stress/strain value obtained from the CG Model-1 is very close to that from MD simulations, those from CG Model-2 and CG Model-3 are slightly higher than those from MD simulations (Figs. 3 and 4).
Unlike a typical smooth stress–strain plot of bulk single crystals, these stress–strain curves are composed exclusively of elastic loading segments followed by discrete strain bursts, a phenomenon observed in experiments (Brinckmann et al., 2008). These bursts have been found to be correlated with the avalanche of dislocations activated in the glide planes. The amplitude of those bursts in the stress–strain curves by CG models is larger than that in MD simulations. This may be caused by the assumption of the linear shape function employed in CG models, and/or by the Nose–Hoover (NVT) algorithm in MD simulation to enforce constant temperature, which seems to have an effect of attenuating the frequency of the stress fluctuations. It should be noted, however, that the stress–strain curves obtained from CG simulations agree well with those from MD simulations in an average sense up to a strain $\varepsilon \approx 0.03$ for CG Model-1 and $\varepsilon \approx 0.025$ for CG Model-3. Moreover, the specimen size dependence from MD is captured by CG modeling.

Fig. 5 plots mesh deformation from the CG simulations. Under tensile loading, we see that the finite elements in the CG models are stretched to accommodate the elastic deformation. Meanwhile, neighboring elements are sliding along the {1 1 1} slip planes (red lines are drawn to assist visualization) corresponding to the dislocation migration and formation of stacking faults.

Fig. 6 presents a strain sequence of snapshots of atomic arrangements of the largest specimen with the coarsest mesh, Model-3, comparing CG and MD simulations. Fig. 7 presents the evolution of the dislocations (blue atoms) and stacking faults (red atoms) visualized through the centrosymmetry parameter (Kelchner et al., 1998) implemented in AtomEye (Li, 2003). It is seen that dislocations nucleate at $\varepsilon \approx 0.005$ and are then emitted from the notch tips, leaving stacking faults behind, with
Fig. 5. Mesh deformations from CG simulations: (a) CG Model-1 at \( \varepsilon = 0.026 \) (125 atoms per element); (b) CG Model-2 at \( \varepsilon = 0.018 \) (729 atoms per element); and (c) CG Model-3 at \( \varepsilon = 0.017 \) (1331 atoms per element) (red lines are drawn to assist visualization) (for interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

Fig. 6. Strain sequence of snapshots of atomic arrangements in Model-3. (a) Atomic arrangements from CG simulation (1331 atoms per element), Model-3. (b) Atomic arrangements from MD simulation, Model-3.
the dislocation line being perpendicular to the (1 1 0) surface plane, a process that has been observed in all of the simulations conducted in this work. Comparing Figs. 6a and b, we see that the CG simulations have produced similar dislocation structures and stacking faults to those of MD simulations. The CG simulation results start to diverge from MD results at \( \varepsilon \approx 0.01 \) when the MD notch tips begin to blunt, while the CG tips do not. This is likely a consequence of the uniform coarse mesh, the assumption of a linear shape function employed in the CG method, and the occurrence of dislocation glide along the element interfaces.

4.2. Dislocation–dislocation interactions

To investigate the dynamics of dislocation–dislocation interactions, two computer models of notched single-crystal copper specimens with symmetric geometry and boundary conditions are constructed with different FE mesh sizes, as shown in Fig. 8. The models contain 79,750 atoms (25 nm \( \times \) 12 nm \( \times \) 2.3 nm, noted as CG Model-4) and 849,178 atoms (56 nm \( \times \) 25 nm \( \times \) 5.4 nm, noted as CG Model-5), respectively. Both are discretized into 638 elements with element surfaces.
The stress–strain curves from CG Model-4 and MD are compared in Fig. 9. It is seen that the stress–strain curve produced from CG simulation agrees well with MD simulation on average.

Fig. 10 shows the atomic rearrangements, dislocation structures (blue atoms), and stacking faults (red atoms) simulated by CG and MD for Model-4, respectively. It is seen that dislocations are emitted from the notch tips and propagate to the specimen interior. Although the geometry, loading and boundary conditions of the computational model are perfectly symmetric, we see that the dislocation nucleation and migration is not symmetric. When the strain reaches $\varepsilon \approx 0.0215$ in the CG simulation, or $\varepsilon \approx 0.0205$ in the MD simulation, dislocations emitted from the two notch tips interact and appear to form what is known as a Lomer–Cottrell or stair-rod lock (Weertman and Weertman, 1992; Hirth and Lothe, 1992; Yamakov et al., 2003). Both the CG and MD simulations have found that this lock hinders further glide on the two slip planes and provides a barrier to other dislocations. Thereafter, we observe dislocations move towards the surface of the specimen along [1 1 0] direction in the CG simulation, while the notch tips start to blunt in the MD simulation. Again, the notch tip blunting phenomenon is not reproduced in CG simulation, indicating the need for mesh refinement in the vicinity of the tips of the notches.

Fig. 11 shows the atomic rearrangements, dislocations (red atoms) and stacking faults (blue atoms) from MD and CG simulations of Model-5; 1331 atoms are embedded within each element. Although a much coarser mesh has been employed in this CG simulation, the same phenomena associated with dislocation interactions are observed. This leads us to conclude that the CG method can capture the phenomenon of Lomer–Cottrell locks formed by dislocation interactions over this range of mesh size.

4.3. Dislocation–stacking fault interactions

To simulate the dynamics of dislocation–stacking fault interactions in the early stages of plastic deformation, a CG model of a notched single-crystal copper specimen with asymmetric notches (the notch size on the right side is larger than that on
the left-hand side) is constructed, as shown in Fig. 12. The model (noted as CG Model-6, 56 nm × 25 nm × 5.4 nm) contains 857,164 atoms. It is discretized into 644 elements with each element containing 1331 atoms. The stress–strain curve from CG is compared with MD results in Fig. 13.

Figs. 14 and 15 show snapshots of atomic rearrangements, dislocation structures (blue atoms), and stacking faults (red atoms) from CG and MD simulations for Model-6. Compared with MD simulation results, the CG simulation captures the essential features of dislocation migration and formation of stacking faults. However, the thickness of the stacking fault ribbons from the CG simulations is found to be 2 atomic layers in Figs. 14b, c, but the thickness of the ribbons in MD simulations is nonuniform, as shown in Figs. 15b, c. Such differences between CG and MD simulations are believed to be caused by the assumption of linear finite element shape functions. As a result of this assumption, the CG simulations cannot fully reproduce the incipient stages of stacking fault formation observed in MD.

Figs. 16 and 17 present 3D views of the dynamic dislocation interaction processes (blue atoms) and stacking faults (red atoms) from CG and MD simulations. It is seen from Figs. 16b and 17b that when the dislocation approaches the stacking faults, its elastic field unfolds the stacking fault layers. In Figs. 16c and 17c, we see that the stacking faults have been split into two segments. This is also consistent with the observations reported in a previous atomistic simulation by Yamakov et al. (2003), and in both direct atomistic simulation and dislocation dynamics simulation of FCC crystals by De Koning et al. (2003). The mechanism of the splitting was traced to a spontaneous nucleation of new partials within the stacking faults, clearing the faults and restoring the normal FCC coordination across their area (De Koning et al., 2003).

4.4. Dislocations in a submicron thin sheet specimen

Fig. 18 shows the computer model (Model-7) of a single crystal copper sheet (0.12 μm × 0.1 μm × 8.3 nm) containing ~6 million atoms. The specimen is discretized into 4167 elements with each element containing 1331 atoms. Tensile loading is applied on the two edges of the specimen with all of the other surfaces free. Owing to the large number of atoms involved in this simulation, only a thin slice of this specimen is displayed for dislocation visualization. The extraction of the slice is shown in Fig. 18c.

Fig. 19 shows a series of simulation results for atomic rearrangements, dislocations, and stacking faults for strain values from \( \varepsilon = 0.0076 \) to \( \varepsilon = 0.0221 \). In Fig. 19b, the stacking faults (red atoms) are split by the incoming dislocations (blue atoms), and then allow the dislocations to pass through. In Figs. 19c, d, more and more dislocations are nucleated and stacking fault ribbons are formed as the tensile strain is increased.

At \( \varepsilon = 0.0265 \), dislocations and stacking faults in the specimen are shown in Fig. 20a. Fig. 20b plots the corresponding local stress field showing stress component normal to the (1 1 0) plane, calculated via Eq. (2.19). The dislocation density is not
increased or even slightly decreased although the tensile strain has been increasing. One reason is that some dislocations have moved out of the sample to the surfaces. Another possible reason is that dislocation annihilation has occurred due to interactions between dislocations with opposite Burgers vectors. It is clearly seen in Fig. 20b that, due to nonlocal constitutive

Fig. 11. Strain sequence of snapshots of atomic arrangements, dislocations and stacking faults. (a) Results from CG simulation (1331 atoms per element), Model-5. (b) Results from MD simulation, Model-5.

Fig. 12. CG Model-6: (a) the specimen, (b) FE model; and (c) boundary conditions.

increased or even slightly decreased although the tensile strain has been increasing. One reason is that some dislocations have moved out of the sample to the surfaces. Another possible reason is that dislocation annihilation has occurred due to interactions between dislocations with opposite Burgers vectors. It is clearly seen in Fig. 20b that, due to nonlocal constitutive
relation (i.e., internal force–displacement relationship) employed in the CG simulation, the stress field does not exhibit the singularity predicted by the classical local elastic field theory. Rather, around each dislocation core, the stress fields exhibit peak value at distances in the range of several angstroms and decrease rapidly within the core itself.

5. Summary and discussion

This paper has presented a new coarse-graining methodology for dynamic simulation of dislocation nucleation and glide, with application to FCC crystals. The methodology combines an atomistic formulation of balance equations and a modified
finite element method employing rhombohedral-shaped 3D solid elements. As such, it is able to predict dislocation nucleation and splitting into partial dislocations in a manner that mimics atomistic simulations. Seven CG computer models with different mesh sizes and/or different geometries were utilized to test the accuracy and efficiency of the CG method relative to fully atomistic models in modeling the dynamics of dislocations. The CG method has predicted the threshold
stress/strain for the dislocation nucleation and specimen size effect in good agreement with that obtained by fully atomistic models, and has also given good estimates for average stress–strain responses of notched specimens under tension. Although the majority of the degrees of freedom (more than 99%) of the simulated atomistic system has been eliminated by coarse-graining, the CG simulations have captured key phenomena of dislocation dynamics, including dislocation nucleation and migration, formation of stacking fault ribbons, dislocation–dislocation interactions, dislocation–stacking fault interactions, and the formation of stair-rod dislocations, not in exact correspondence, but similar to that from MD simulations without strong evidence of FE mesh-size dependence. In the simulation of a submicron-sized specimen under tension, a significant number of dislocations have been nucleated and multiple stacking fault ribbons are formed simultaneously. It appears that the CG method is applicable to mesoscale simulations and complex dislocation activities such as dislocation annihilation, dipole formation, junction formation, etc.

Most contemporary coarse-graining methods begin with the determination of the total potential energy of a system as a function of the degrees-of-freedom. A Hamiltonian or an effective potential is constructed or numerically obtained in terms of

**Fig. 19.** Strain sequence of atomic arrangements, dislocations and stacking faults from CG Model-7.
representative atoms or a group of atoms. The coarse-grained Hamiltonian is then minimized to find the equilibrium state (Tadmor et al., 1996, 1999; Abraham et al., 1998; Knap and Ortiz, 2001; Muller-Plathe, 2002; Dupuy et al., 2005), or used to derive the coarse-grained equations of motion to model the dynamics of the systems (Rudd and Broughton, 1998). This paper has presented a new coarse-graining methodology. The fundamental difference between this new method and existing coarse-graining or multiscale methods is that we start with the dynamics of atoms, derive the exact field representation of balance equations from atomic variables, and then solve for the dynamic response of the coarse-grained system.

The dislocation dynamics (DD) method is the most popular CG method employed in simulation of dislocations (Amodeo and Ghoniem, 1990a, b; Van der Giessen and Needleman, 1995; Zbib et al., 1998; Rhee et al., 1998; Schwarz, 1999; Ghoniem et al., 2000; Devincre et al., 2001). The DD method has been successfully employed in the study of a host of important problems in dislocation mechanics and has the potential of directly connecting the physics of dislocations with the strength and strain hardening of crystals. Fundamentally different from the present CG method, DD focuses on individual dislocations, and explicitly simulates the migration, multiplication and interaction of discrete dislocation lines; accordingly, the number of active degrees of freedom can increase dramatically during the course of the simulation (Arsenlis et al., 2007). The focus of DD is typically placed on mesoscopic scales associated with dislocation substructures, since the theory does not consider regions of the domain with full atomic resolution. The present CG method is intended to address problems involving mesoscale description of dislocation structure (e.g., pileups) and associated long range fields with certain regions of interest (e.g., interfaces) treated with full atomic resolution to take advantage of predictive capabilities of MD, as in the aforementioned CADD formalism.

The only constitutive law involved in this formulation is the interaction of atoms, the atomistic counterpart of constitutive relations. Therefore, in the finite element implementation, connectivity between finite elements is not required even with standard finite element method, similar to the key feature of cohesive zone model (Needleman, 1987). By using a traction–displacement relation between finite elements, the cohesive zone model can simulate separations of finite elements and has therefore enjoyed a great popularity in simulations of crack propagation. One major difference between the present formulation and the cohesive zone model is that we use the same constitutive relation between finite elements as well as within a given finite element. Thus, nucleation of dislocations or initiation of cracks (i.e., separation of finite elements) would emerge naturally as a direct consequence of the governing equations, i.e., the balance equations supplemented by internal force fields.

Note that when the balance equation of linear momentum is expressed in terms of internal force density, as in Eq. (2.23), instead of the divergence of stress as is in the usual continuum mechanics representation, it then becomes very similar to the governing equation of Peridynamics (Silling, 2000), except that we have a temperature gradient term in the balance equation of linear momentum. On the other hand, since there is a temperature gradient term in the balance equation of linear momentum, together with the energy equations, the present method can take account of finite temperature or solve for local temperature, thereby achieving thermo-mechanical coupling.

A number of numerical methods have been developed using discontinuous basis functions in the finite element implementation to accommodate discontinuities. Popular methods include the discontinuous Galerkin (DG) method and the extended finite element method (XFEM). In the XFEM, discontinuities are incorporated into the continuum model using the enrichment of the standard FEM approximation by the Heaviside step function (Gracie and Belytschko, 2009). In the DG method, the approximated displacements are discontinuous across finite elements. The DG method was developed for high-order accuracy on unstructured meshes, local hp-refinement, and high parallel efficiency. It also provides a framework that can naturally incorporate the cohesive zone model or XFEM for simulation of fracture (Stan, 2008; Abedi et al., 2010; Gracie et al., 2007). Different from many continuum models that require special numerical treatment for simulation of discontinuous phenomena, the governing equations of the present CG model can be recast in a mathematical form that permits discontinuities and hence facilitates simulation of the initiation and evolution of discontinuities.
Comparing with MD simulations, the present coarse-graining approach is more efficient (0.6% in terms of degrees of freedom and < 2% in terms of computer operations with current numerical algorithms for the largest model in this work), yet it is still able to capture key phenomena of the dynamics of dislocations. Constrained by the assumptions of cooperative deformation of unit cells within a finite element and homogeneous temperature, the thermal fluctuation of atoms is smoothed out. As a result, the CG simulations yield a description of dislocation dynamics that are less accurate than, but qualitatively comparable to, MD results.

The accuracy of the coarse-grained simulation depends on the constitutive relations, that is, the underlying interatomic potential or the force fields, in addition to the numerical implementation method, including the size and shape of the finite elements. The rhombohedral-shaped element enables simulation of dislocations glide between elements on (1 1 1) or (1 1 ¯ 1) slip systems along element boundaries. However, according to the standard Thompson tetrahedron representation of dislocations in FCC crystals, such a rhombohedral-shaped element still cannot completely capture all possible dislocation kinematics. For example, climb or cross-slip would be constrained in the current CG models implemented with only rhombohedral-shaped elements. Also, as a result of the coarse mesh at notch tips, the CG simulations are unable to model crack tip blunting, excessive nucleation frequency, and consequently, CG simulation results diverge from MD at large strains. Future work will include more sophisticated force fields to better describe stacking fault energy, such as EAM (Horstemeyer et al., 2001; Mishin et al., 2001), tetrahedral-shaped elements to admit more dislocation kinematics, more advanced shape functions to include formation of stacking faults within finite elements, adaptive remeshing to distinguish regions of higher defect concentration from coarse-grained regions, and/or linking to fully atomistic model in a concurrent atomistic–continuum simulation. Another future direction for the new CG method is to develop a corresponding parallel code for simulation of micron to millimeter-sized specimens and mesoscopic phenomena such as planar dislocation arrays and cell formation. In addition, this paper only presents a special case of systems with a homogeneous temperature field at a very low temperature. It should be noted that dealing consistently with finite temperatures in coarse-grained modeling is not necessarily straightforward. Future work will include the effect of thermal fluctuation for systems at high temperature and also thermo-mechanical coupling for large plastic deformation and for dynamic crack propagation.

Acknowledgements

This work was supported by National Science Foundation under Award nos. CMMI-0758265 (Tucker and McDowell), CMMI-0824688, CMMI-0855795, and DARPA under Award no. N66001-10-1-4018 (Xiong and Chen). Simulations were performed at the High Performance Computing Center at University of Florida with technical support from Dr. Charles Taylor. Discussions of this work with Dr. Jonathan Zimmerman of Sandia National Laboratories and Professor William Curtin from Brown University are gratefully acknowledged.

References
