Multiscale modeling and simulation of single-crystal MgO through an atomistic field theory

Liming Xiong, Youping Chen *

Department of Mechanical and Aerospace Engineering, University of Florida, Gainesville, FL 32611, USA

Abstract

The present work is concerned with the application of an atomistic-continuum field theory (AFT) in modeling and simulation of crystalline materials. Atomistic formulation of the field theory and its finite element implementation are introduced. Single-crystal MgO under mechanical loading is modeled and simulated. With a coarse mesh, the field theory is shown to be able to simulate dynamic and nonlinear behavior of multi-atom crystalline materials without the need of additional numerical treatments. Reducing the finite element mesh to the atomic scale, i.e., the finite element size is equal to the size of the primitive unit cell, atomic-scale critical phenomena, including dislocations nucleation and motion, have been successfully reproduced.

1. Introduction

The past decades have seen the explosive growth of interest in theory and modeling of microscale, nanoscale and multiscale material behavior. One of the most popular concurrent multiscale modeling approaches is replacing the finite element (FE) equations of motion on regions of the mesh that are atomic-sized with MD equations of motion and implementing a hand shaking region between the MD and FE regions (Broughton et al., 1999; Cai et al., 2000; Wagner and Liu, 2003; Xiao and Belytschko, 2004; To and Li, 2005). One unsolved problem with this method that combines several theoretical descriptions is the phonon scattering and wave reflection at the numerical interfaces between atomistic models and continuum mechanics. A typical popular bottom-up approach is the quasicontinuum (QC) method developed by (Tadmor et al., 1996). In QC method, a crystalline solid is discretized into a set of nodes. There is a group of atoms embedded within each node. The classical continuum mechanics governing equations are then solved at the continuum level to obtain the deformation gradient of each node. Based on the deformation gradient, the positions of atoms within the nodes are determined using the conjugate gradient method according to the Cauchy–Born rule. The QC method reproduces the result of standard lattice static techniques. Through a statistical coarse graining procedure, a technique for simulation of the mechanics of micron-scale solid systems, coarse-grained molecular dynamics (CGMD), is developed to capture the important atomistic effects without the computational cost of conventional molecular dynamics (Rudd and Broughton, 1998). Another idea that has recently been pursued is a general multiscale method using the framework of the heterogeneous multiscale method (HMM), in which both the atomistic and the continuum models are formulated in the form of conservation laws of mass, momentum and energy (Li and E, 2005). For a more complete review of available multiscale methods, see Curtin and Miller (2003).

It is also worthwhile to mention the well-established microcontinuum field theories developed by Eringen and Suhubi (1964). These microscopic continuum theories are the logical extensions of the classical field theories for the applications in microscopic space and short time scales, and may be considered to be the most successful top-down multiscale models. The fundamental departure of the microcontinuum theories from the classical counterpart is that the former are continuum models embedded with microstructure for the purpose of describing the microscopic motion and deformation. Micromorphic Theory (Eringen and Suhubi, 1964; Eringen, 1999) treats a material as a continuous collection of deformable particles, each particle possessing finite size and inner structure. Upon assumptions of a small deformation and slow motion, Micromorphic Theory can be reduced to Mindlin’s Microstructure Theory (1964). When the microstructure of the material is considered as rigid, Micromorphic Theory then reduces to the Micropolar Theory (Eringen, 1965). Assuming a constant microinertia, the Micropolar Theory is identical to the Cosserat Theory (1909). Eliminating the distinction of macromotion of the particle and the micromotion of its inner structure, it results in the Couple Stress Theory that considers the effect of the gradient of the rotational part of the deformation (Toupin, 1962; Mindlin, 1964). A full gradient of strain was considered in the Second Gradient Theory by...
Mindlin and Eshel (1968). When the particle reduces to the mass point, all of the microcontinuum theories go back to the classical continuum mechanics.

The microcontinuum theories or the generalized continuum theories mentioned above may be considered as two-scale continuum models, in which the deformation is expressed as a sum of macroscopic continuous deformation and an internal microscopic deformation within the inner structure of the material points. Chen et al. (2003) have examined the physical foundation of those microcontinuum theories from the viewpoints of phonon dispersion relations, and concluded that the applicability of those microcontinuum theories is limited because of the continuum assumption of the microstructure. Motivated by the applicability and limitation of microcontinuum theories as well as by a bottom-up formalism of linking atomistic model to continuum descriptions by Irvine and Kirkwood (1950) and Hardy (1982), in a series of theoretical papers, a new continuum field theory has been formulated by Chen and her coworkers. Continuous local densities of fundamental physical quantities (Chen and Lee, 2005) have been formulated by Chen and her coworkers. Continuous local densities of fundamental physical quantities (Chen and Lee, 2005) in an atomic system are derived. By decomposing the atomic-scale deformation into the homogeneous lattice deformation and an inhomogeneous internal atomic deformation (Fig. 1), and also decomposing momentum flux and heat flux into homogeneous and inhomogeneous parts, the field representation of conservation laws (Chen and Lee, 2005) at the atomic scale has been formulated. Subsequently, a continuum field representation of atomistic systems is obtained, leading naturally to an atomistic-continuum field theory (Chen and Lee, 2005, 2006; Chen, 2006; Chen et al., 2006a,b), in which a material is viewed as a continuous collection of lattice points, while embedded within each lattice point is a group of discrete atoms, cf. Fig. 1. In AFT, the lattice deformation is homogenous and continuous, but the internal deformation is inhomogeneous.

This paper is concerned with the applications of the newly formulated AFT in the simulation of microscopic material behavior. The material to be investigated is single-crystal MgO. Commonly, due to its simple rocksalt structure and well-defined deformation properties, MgO is suitable to be used as a testing material for understanding the deformation mechanism of metal oxides. It is also an ideal choice for the purpose of the present study. Following this introduction, the atomistic formulation of AFT will be briefly introduced in Section 2 and the finite element implementations will be developed in Section 3. Coarse-scale and atomic-scale simulation results will be presented in Sections 4 and 5. We will conclude this paper with a brief summary and discussion in Section 6.

2. Formulation of the atomistic field theory

In contrast with the classical statistical mechanics approaches or the existing formalisms that link atomic variables to continuum field variables (Hardy, 1982), AFT views a crystalline material as a continuous collection of lattice points (or lattice cells) but embedded within each lattice point is a group of atoms. The local density of any measurable phase-space function $A(R^k, V^k)$ can thus be generally defined as

\[
\rho(x, y) = \sum_{k=1}^{n} \sum_{i=1}^{i} A(R^k, V^i) \delta(R^k - x) \delta(\Delta R^k - y)
\]

with normalization conditions

\[
\int_{V} \delta(R^k - x) dx = 1 \quad (k = 1, 2, 3, \ldots, n).
\]

Eq. (2) implies that over the entire physical space all the unit cell can be found. Then, for each unit cell $k$, the second $\delta$-function in Eq. (1), $\delta(\Delta R^k - y^k)$, identifies $y^k$ to be $\Delta R^k$. It follows

\[
\int_{V} \delta(R^k - x) \delta(\Delta R^k - y^k) dx = 1 \quad (k = 1, 2, 3, \ldots, n) \quad (x = 1, 2, \ldots, v).
\]

Here, the superscript $kx$ refers to the $x$th atom in the $k$th unit cell, $(x = 1, 2, \ldots, v) (k = 1, 2, 3, \ldots, n), R^k$ is the mass center of the $k$th unit cell and $V^k$ is the velocity vector of the $k$th atom, respectively; $\Delta R^k$ is the atomic position relative to the lattice, respectively, $V$ is the volume of the whole system. The localization functions can be a Dirac delta function (Irvine and Kirkwood, 1950), or a Gaussian distribution function, or any non-negative function that is peaked at $x = R^k$ and tends to zero as $|x - R^k|$ becomes large (Hardy, 1982). It has been proved (Hardy, 1982; Chen and Lee, 2005) that the forms of the conservation equations are independent of the choices of the form of localization function.

Defining the averaged quantities over the time interval $\Delta t$ as

\[
\bar{a}(x, y^k) = \frac{1}{\Delta t} \int_{0}^{\Delta t} \sum_{k=1}^{n} A(R^k(t + \tau), \Delta R^k(t + \tau)) \delta(R^k - x) \times \delta(\Delta R^k - y^k) d\tau \equiv \langle A^k \rangle,
\]

following Eqs. (1) and (4), the time-interval averaged continuous local mass density $\rho^k$, linear momentum density $\rho^k(\mathbf{v} + \Delta \mathbf{v})$, internal energy density $\rho^k U^k$, and temperature $T^k$ can be defined as

\[
\bar{\rho}^k = \rho(x, y^k, t) \equiv \langle \sum_{k=1}^{n} m^k \delta(R^k - x) \delta(\Delta R^k - y^k) \rangle,
\]

\[
\bar{\rho}^k(\mathbf{v} + \Delta \mathbf{v}) \equiv \langle \sum_{k=1}^{n} m^k \mathbf{V}^k \delta(R^k - x) \delta(\Delta R^k - y^k) \rangle.
\]

\[
\bar{\rho}^k U^k \equiv \langle \sum_{k=1}^{n} \frac{1}{2} m^k (\mathbf{V}^k)^2 + U^k \delta(R^k - x) \delta(\Delta R^k - y^k) \rangle.
\]

\[
T^k \equiv \frac{\Delta V}{3 k_B} \sum_{k=1}^{n} \sum_{i=1}^{i} m^k \langle \frac{1}{2} \mathbf{V}^k \delta(R^k - x) \delta(\Delta R^k - y^k) \rangle.
\]

where $\mathbf{V}^k = \mathbf{V}^k - \mathbf{v} - \Delta \mathbf{v}$ is the difference between the phase-space velocity and the local velocity field, $k_B$ is the Boltzmann constant; $\Delta V$ is the volume of material point $x$, or the volume of primitive unit cells, $U^k$ is the potential energy of the $k$th atom.

As exact consequences of Newton’s laws, the time evolution laws of conserved quantities have been obtained to be (please see Chen and Lee, 2005 for detailed derivation)

![Fig. 1. General picture of a multi-atom crystal structure.](image-url)
\[
\frac{d\rho^a(x)}{dt} + \rho^a(x)(\nabla_x \cdot \mathbf{v}(x) + \nabla_y \cdot \Delta \mathbf{v}^y(x)) = 0, \tag{9}
\]
\[
\rho^a(x) \frac{d}{dt} \mathbf{v}(x) + \Delta \mathbf{v}^y(x) = \nabla_x \cdot \mathbf{t}^a(x) + \nabla_y \cdot \mathbf{t}^y(x) + \mathbf{f}_{\text{ext}}^a(x), \tag{10}
\]
\[
\rho^a(x) \frac{d^2 \mathbf{v}^y(x)}{dt^2} = \nabla_x \cdot \mathbf{q}^a(x) + \nabla_y \cdot \mathbf{q}^y(x) + \mathbf{t}^a(x) \cdot \nabla_x \mathbf{v}(x) + \Delta \mathbf{v}^y(x), \tag{11}
\]
where \( \mathbf{f}_{\text{ext}}^a(x) \) is the external force density, \( \mathbf{t}^a(x) \) and \( \mathbf{t}^y(x) \) are the homogeneous and inhomogeneous parts of the atomic stress (momentum flux density), which further consist of a kinetic part that is related to temperature, and a potential part that is related to the internal force density (Chen and Lee, 2005; Hardy, 1982); \( \mathbf{q}^a(x) \) and \( \mathbf{q}^y(x) \) are the homogeneous and inhomogeneous parts of heat flux, which also further consist of kinetic and potential parts (Hardy, 1963).

Substituting the relationships between the kinetic stress and temperature as well as between the potential stress and the internal force density (for detailed derivations please see Chen and Lee, 2005) into Eq. (10), we obtain
\[
\rho^a(x) \frac{d}{dt} \mathbf{v}(x) + \Delta \mathbf{v}^y(x) = \frac{m^2 k_b}{MV^2} \nabla_x \mathbf{t}^a(x) - \mathbf{f}_{\text{int}}^a(x) + \mathbf{f}_{\text{ext}}^a(x). \tag{12}
\]
For material systems that involve pair atomic interactions and below half melting temperature, the average internal force density usually takes the following form as
\[
\mathbf{f}_{\text{int}}^a(x) = \int_{\Omega(x')} \sum_{j=1}^n \mathbf{f}(\mathbf{u}^j(x), \mathbf{u}^j(x'))d\mathbf{x}', \tag{13}
\]
where \( \Omega(x') \) is the domain associated with the material point \( x' \). It is noted that the internal force density \( \mathbf{f}_{\text{int}}^a(x) \) is a nonlocal and nonlinear function of the averaged atomic displacements or positions. It can be obtained through fitting to the experimental measurements or first principle calculations. In this paper, for the ionic MgO crystal, the internal force density is derived from the combination of the long range electrostatic Coulomb potential and the Buckingham short range pair potential (Xiong et al., 2006) with the material parameters taken from the literature (Grimes, 1994).

The mass density is defined mathematically in accordance with the continuum concept by the limit \( \rho = \lim_{\Delta V \to 0} V / \Delta V \). In lattice systems, the smallest allowable physical volume is the volume of a primitive unit cell. The mass density of the \( x \)th atom at a material point \( x \) is thus given as
\[
\rho^a(x) = m^2 / \Delta V. \tag{14}
\]
Using the atomic mass \( m^2 \) as a material constant and considering that the volume of the unit cell \( \Delta V \) varies during the deformation, the conservation law of mass will be automatically satisfied. Eq. (14) can thus replace the traditional conservation equation of mass. For systems with a given constant temperature field or constant temperature gradient, the temperature would behave like a surface traction on the boundary or a body force (noted as \( \mathbf{f}_{\text{ext}}^b(x) \)) in the interior of the material, then Eq. (12) can be written as
\[
\rho^a(x) \frac{d}{dt} \mathbf{u}^a(x) = \mathbf{f}_{\text{int}}^a(x) + \mathbf{f}_{\text{ext}}^a(x) + \mathbf{f}_{\text{ext}}^b(x), \tag{15}
\]
where \( \mathbf{u}^a(x) = d [\mathbf{v}(x) + \Delta \mathbf{v}^y(x)] \). Together with Eqs. (13)–(15) can serve as the governing equation to solve for the averaged atomic displacement field, and consequently, atomic-scale properties.

3. Finite element implementations

For the purpose of large-scale simulation of collaborative materials behavior, we seek an approximate solution to Eq. (15) through interpolation using the concept of shape functions
\[
\mathbf{u}^a_i(x) = \Phi_i(x) \mathbf{U}^a_i \quad \text{or} \quad \mathbf{u}^a_i(x) = \Phi_i(x) \mathbf{U}^{a,n} _i, \quad \zeta = 1, 2, \ldots n, \quad i = 1, 2, 3, \tag{16}
\]
where \( \mathbf{u}^a_i(x) \) stands for the approximation of the atomic-scale displacement field within elements, \( \mathbf{\Phi}_i(x) \) is the shape function, and \( \mathbf{U}^{a,n} _i \) is the displacement of the \( x \)th atom embedded within the \( n \)th node. Following the standard procedure of the Galerkin method (Belytschko et al., 2000), the weak form of Eq. (12) is written as
\[
\int_{\Omega(x')} \mathbf{\Phi}_i(x) \left( \frac{d^2 \mathbf{u}^a_i(x)}{dt^2} - \frac{\mathbf{f}_{\text{ext}}^a(x)}{\rho^a(x)} \right) dx - \int_{\Omega(x')} \mathbf{\Phi}_i(x) \frac{\partial \mathbf{f}_{\text{int}}^a(x)}{\partial t} dx = 0, \tag{17}
\]
i.e.,
\[
\int_{\Omega(x')} \mathbf{\Phi}_i(x) \frac{d}{dt} \mathbf{t}^a(x) - \int_{\Omega(x')} \mathbf{\Phi}_i(x) \mathbf{f}_{\text{ext}}^a(x) dx + \int_{\Omega(x')} \mathbf{\Phi}_i(x) \frac{d}{dt} \mathbf{f}_{\text{int}}^a(x) dx = 0. \tag{18}
\]
Then the matrix form of Eq. (17) can be written as
\[
\mathbf{M} \mathbf{u} = \mathbf{f}_{\text{ext}} + \mathbf{f}_{\text{int}} + \mathbf{f}_{\text{rem}}, \tag{19}
\]
where
\[
\mathbf{M} = \int_{\Omega(x')} \mathbf{\Phi}_i(x) \mathbf{\Phi}_j(x) dx, \tag{20}
\]
\[
\mathbf{F}_{\text{int}}(\mathbf{U}) = \int_{\Omega(x')} \mathbf{\Phi}_i(x) \sum_{j=1}^n \mathbf{f}(\mathbf{\Phi}_j(x) \mathbf{U}^a_j, \mathbf{\Phi}_j(x) \mathbf{U}^{a,n} _j) dx, \tag{21}
\]
\[
\mathbf{F}_{\text{ext}} + \mathbf{F}_{\text{rem}} = \int_{\Omega(x')} \mathbf{\Phi}_i(x) \frac{d}{dt} \mathbf{f}_{\text{int}}^a(x) + \frac{d}{dt} \mathbf{f}_{\text{rem}}^a(x) dx. \tag{22}
\]
Eqs. (20)–(22) can be evaluated through numerical integrations such as Gauss integration or nodal integration. Compared with the Gauss integration procedure, nodal integration is less complex and more efficient, but usually leads to instability and needs additional numerical treatments in the finite element implementation of classical continuum mechanics (Puso et al., 2008). In this work, the nodal integration scheme is implemented because of its efficiency and simplicity and we believe that the nonlocal character of the atomistic field theory can bring in both accuracy and convergence properties. The central difference method is used for solving the governing equation (19) and the time step is 1 fs.

Since AFT has been constructed in terms of local densities, in the finite element implementations of AFT, different meshes can be used in the regions of different concerns. When coarse mesh is used, the majority of the degrees of freedom can be eliminated, hence, the computational cost can be reduced. When the finest mesh is used, the positions of the finite element nodes coincide with lattice sites, and the computational model becomes identical to a full MD model. In this work, for nanometer-sized single-crystal MgO, coarse mesh is employed to characterize the mechanical properties as presented in Section 4. In Section 5, the finest mesh is implemented to capture the atomistic material behavior such as dislocations nucleation and motion.

4. Coarse-scale simulations

4.1. Wave propagation

Under a uniaxial compressive loading, with a constant velocity of about 10,000 m/s, the boundary displacement is applied on the two ends of an MgO sample (5 nm × 5 nm × 10 nm). The displace-
ment is increased to 2 nm in a linear ramp over 20 fs. Thereafter, the displacements on the two ends are held as constant. Fig. 2 shows the computational model, loading history and the boundary conditions. Uniform 3D 8-node brick-type element is used. There are 96 elements and 275 nodes in the FE model. There are 41,192 atoms if it is simulated by a fully MD simulation. Approximately, the number of degrees of freedom involved in AFT is about 5% of that of MD.

Fig. 3 shows the contour plots of stress wave propagations and snapshots of atomic arrangements in the single-crystal MgO. It is observed that upon the compressive loading, very strong compressive normal stresses develop just beneath the boundaries. The normal stresses originate from the two ends, propagate to the middle of the sample, and then they meet and separate. The propagation is largely along the z direction and no propagation of $\sigma_{zz}$ in the x or y direction is observed in Fig. 3. It is found that $\sigma_{zz}$ is featured with a compressive stress in the centre and a tensile stress on the surface of the specimen.

In this example, through the simulations of the complete period of wave propagation, meeting, separation and reflection, the robustness and stability of the finite element implementations using nodal integration is demonstrated.

4.2. Uniaxial tension and compression

Under uniaxial tension and compression, a small MgO specimen (3 nm × 3 nm × 5 nm, 8424 atoms) is discretized into 96 elements. There are 175 finite element nodes in the computational model. Thus the number of the degrees of freedom involved in AFT is about 17% of that of MD. In the simulation of MgO under tension, displacement controlled boundary conditions with a constant velocity of 100 m/s are applied on the two ends and the total loading time is 5 ps (Fig. 4b). For the specimen under compressive loadings, three loading cases are simulated. With the same constant velocity, the boundary displacement is increased to 0.25 nm (Case-A), 0.40 nm (Case-B) and 0.50 nm (Case-C) in a linear ramp over 2.41 ps (Case-A), 3.87 ps (Case-B) and 4.83 ps (Case-C) and then the displacement on the two ends are held as constant (Fig. 4c).

The stress–strain curve obtained through the simulation of MgO under tension is plotted in Fig. 5. Here, stress is computed through the average of the local stresses calculated within each unit cell. The stress–strain curve shows a rapid increase in the stress up to the maximum tensile strength followed by a sudden drop when the specimen is going to fail by a localized deformation. This is similar to the conventional tensile testing: the stress–strain curve is essentially smooth with a linear slope within the region of elastic deformation. Both the linear elastic range and the yield point are visible. Young's modulus can be estimated as 200 GPa, which is lower than the bulk experimental or first principle value of 250 GPa. Yield strength is about 11.2 GPa and the yield strain is about 0.08. Those values are close to what has been reported in the previous MD simulation results (Xiong et al., 2006). But here what we like to emphasize is that the stress–strain curve obtained...
from AFT is smoother than that from MD simulation. The reason is that AFT is in terms of the time-interval averaged quantities. This is one major difference between the field representations of the many-body problem and MD simulations: MD solves for the instantaneous quantities first and then obtains the averaged quantities through statistical averaging, while the field theory solves directly for the averaged quantities. The procedure of taking the time-interval averages in MD or ensemble averages in the statistical mechanics is thus eliminated.

For the MgO specimen under uniaxial compression, the evolutions of the averaged compressive stresses $\sigma_{zz}$ are plotted in Fig. 6, and the mesh deformations are plotted in Fig. 7. The vertical axis in Fig. 6 only stands for the magnitude of stress, which actually should be negative because of the compressive loading. It is seen that in the smallest loading case (green line, Case-A), the compressive stress increases linearly with the applied displacement in the loading stage. And then the stress remains as a constant at the holding stage because the deformation in this case is within the limit of elastic region. Consequently, the crystal remains stable and perfect in Case-A. For the other two larger loading cases (blue line for Case-B and black line for Case-C), before the end of the loading stage ($t = 3.87$ ps for Case-B and $t = 4.83$ ps for Case-C), a critical value of $\sigma_c \approx 63.5$ GPa is observed and then followed by a sudden drop. This critical value is close to what is going to be presented in Section 5 (cf. Fig. 10), where the finest mesh is used to discretize the computational model. The evolutions of the mesh deformations and atomic arrangements are plotted in Fig. 7.

5. Atomic-scale simulations

Discretizing the continuous governing equation (15) at primitive unit cell scale, we have a time-interval averaged MD model. In this numerical example, a nanoscale single-crystal MgO speci-
Men subjected to a compressive loading is modeled with the finest mesh to investigate the atomic-scale phenomena. The specimen consists of $7 \times 7 \times 7$ unit cells with eight atoms per unit cell. Different from the coarse mesh which has been used in the previous simulations, in this model, each finite element node corresponds to a lattice point (Fig. 8a). Thus, the number of the degrees of freedom is equivalent to that of the fully MD simulation. A displacement controlled loading is then applied. The loading is similar with what has been applied in the coarse-scale simulations of MgO under uniaxial compression presented in Section 4. With a constant velocity, the boundary displacement is increased to 2.2 Å in a linear ramp over 1.5 ps and then the displacement on the two ends are held as constant (Fig. 8c). Also, in this atomic-scale simulation based on AFT, we used a homogeneous temperature field ($T = 300$ K) for the purpose of comparison with MD simulation results.

Fig. 7. Mesh deformations and atomic arrangements of MgO under compression.

Fig. 8. Computational model: (a) Atomic arrangement, (b) FEM mesh, (c) boundary conditions.

Fig. 9 shows the time evolution of the stress distributions and the corresponding side views of the atomic arrangements. It is seen that there exists a maximum compressive stress (indicated by blue color in Fig. 9) at time equals to 0.72 ps. When the material loses its stability at a critical compressive stress, it yields, and a tensile stress develops (indicated by red color in Fig. 9). Dislocations initiate corresponding to the critical stress point. This explains the sudden drop in the averaged stress curve (cf. Fig. 10) as a result of the development of tensile stress or as a consequence of dislocations nucleation.

Fig. 9. Stress distributions and crystal structure evolution (side view).

Fig. 10. Comparison of the averaged stress of the specimen by AFT and by MD.
Fig. 10 is a comparison between the averaged stress computed by AFT and that by MD. The MD results are obtained by DL-POLY, a general-purpose parallel MD simulation code (Smith and Forester, 2001), and the Hoover constant temperature algorithm (NVT) is employed in the MD simulation with a constant temperature field $T = 300 \text{ K}$. It is seen that the stress curves obtained from these two independent simulations are in good agreement. However, different from the coarse-scale simulation results (Fig. 6, CASE-C), beyond the critical stress point, the averaged stress by AFT oscillates, but the oscillations disappear in time as the enforced constant displacement continues to be held as constant. Note that there is no damping effect incorporated in the simulation code. Therefore, the disappearance of oscillations is not due to dissipation of energy. Rather, we believe that the stress oscillations are the consequence of the motion of dislocations.

Fig. 11 provides the further information of structural evolutions (top view) during the loading stage and the holding stage. It is interesting to see, at the holding stage, while the loading remains as a constant, the atoms continue to move. As a result of the motion of the dislocations (regions within the red circle), the stress oscillates until the dislocations move out of the specimen. We see that steps have been formed, permanent plastic deformations have been generated, and amazingly, the crystal structure becomes ordered again during the holding stage.

6. Summary and discussions

This paper presents the formulation of a multiscale atomistic-continuum field theory and its finite element implementations. Single-crystal MgO under mechanical loading is simulated by the field theory. The major findings of this work are summarized as the following:

(1) Although the nodal integration scheme is well known to be conditional stable in the finite element implementations of classical continuum mechanics, the robustness and stability of the coarse-graining method employing a nodal integration scheme presented in this paper are demonstrated through the simulation of a complete process of dynamic wave propagation.

(2) In the coarse-scale simulations, the majority of degrees of freedom are eliminated and the computational cost is largely reduced. Nevertheless, the essential dynamic and nonlinear large-deformation material behavior has been successfully simulated. With the finest mesh, i.e., the size of finite elements is equal to that of the primitive unit cells, AFT has been shown to be able to simulate the atomic-scale phenomena such as dislocations nucleation and motion.

(3) Mechanical properties such as elastic constant and tensile strength are measured in the coarse-scale simulations of MgO under tension. This shows an advantage of AFT over classical continuum mechanics in predicting the material properties including the constitutive response, while a complicated constitutive relation is needed in classical continuum mechanics-based simulations.

(5) For MgO under compression, both the coarse-scale and atomic-scale simulation results show that there is a critical compressive stress value for the MgO instability. However, atomistic material behavior such as dislocation nucleation and motion has only been captured in the model with the finest mesh. This indicates the need of a concurrent atomistic-continuum model for macroscopic materials involving critical phenomena.

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