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Simulation of dislocation nucleation and motion in single crystal magnesium oxide by a field theory

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Abstract

This paper presents a multiscale field theory and its application in modeling and simulation of the phenomena that take place at atomic scale. Atomistic formulation of a multiscale field theory is introduced. The governing equations for problems with a given temperature are derived. We have modeled and simulated the nucleation and motion of dislocations and the formation of plastic deformation in a nanoscale ionic material MgO. The mechanism of deformation as well as the evolution of the stress has been elucidated. Results are compared with those from molecular dynamics simulations.

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1. Introduction

In the length scales of a nanometer or smaller, one would only see collections of discrete particles, moving under the influence of their mutual interaction forces. Hence, the natural description of microscopic physics is in terms of many-body dynamics. Currently the most popular numerical tool to solve the classical many-body problem is molecular dynamics (MD) simulation. MD simulation in many respects is very similar to real experiments. It consists of three principal steps: (1) construction of a model, (2) calculation of atomic trajectories, and (3) analysis of those trajectories to obtain physical properties. To obtain an observable quantity in MD simulations, one must first of all be able to express this quantity as a function of the positions and momenta of the particles in the system. However, a measured value of $A$, called $A_{\text{meas}}$, is not obtained from an experiment performed at an instant. Rather, the experiment requires a finite duration. During that measuring period, individual atoms evolve through many values of positions and momenta. Therefore the measured value $A_{\text{meas}}$ is generally the phase function $A(r,p)$ averaged over a time-interval $\Delta t$, i.e.

$$A_{\text{meas}}(t) = \frac{1}{\Delta t} \int_0^{\Delta t} A(r(t + \tau), p(t + \tau)) \, d\tau.$$  (1.1)

In equilibrium MD, it is assumed that this time-interval average reliably approximates the time average $\langle A \rangle$,

$$A_{\text{meas}}(t) \approx \langle A \rangle = \lim_{\Delta t \to \infty} \frac{1}{\Delta t} \int_0^{\Delta t} A(r(t + \tau), p(t + \tau)) \, d\tau,$$  (1.2)

which would be obtained from a measurement performed over an essentially infinite duration. Physical properties, such as thermodynamic properties and transport properties, refer only to average behavior. In the past, this was achieved through the theory of statistical mechanics. Averages were constructed by including many similar systems with different initial conditions. By this procedure, starting the system in any initial configuration would yield the same average quantities: this explains the reproducibility of experiments. Therefore, in statistical mechanics, a
A macroscopic field quantity is defined as the ensemble average of an instantaneous dynamical function:
\[ \langle A \rangle \equiv \int_p \int_r A(r,p)f(r,p,t)\, dr\, dp, \]  
where \( f \) is the normalized probability density function, i.e., \( \int_p \int_r f(r,p,t)\, dr\, dp = 1 \).

Eqs. (1.2) and (1.3) distinguish molecular dynamics from statistical mechanics. Statistical mechanics avoids time average by replacing it with an ensemble average by invoking the ergodic hypothesis, which is originally motivated by the inability to actually compute the phase-space trajectory of a real system containing huge number of molecules. As computer power expands, both molecular dynamics simulation and computational statistical mechanics are developing rapidly on many fronts. Science has grown from the days when experiment and theory were the complimentary alternative approaches to understanding. Our goal now is to achieve the correspondence among three alternative descriptions of natural phenomena: theory, experiment, and computer simulation. Experiments are beginning to record atomistic features, usually on a relatively large time scales. Unfortunately even with state of the art computers, those time scales are far beyond the capabilities of current atomistic simulations.

In a series of theoretical papers, a multiscale field theory has been constructed by Chen and her coworkers [2–5]. Local densities of fundamental physical quantities in atomistic systems are derived. By decomposing atomic deformation into homogeneous lattice deformation and inhomogeneous internal atomic deformation, and also by decomposing momentum flux and heat flux into homogeneous and inhomogeneous parts, field representation of conservation laws at the atomic scale has been formulated. The heat flux, atomic stresses, atomic strains, and the atomic stress–strain relations are derived. As a result of the formulation, a field representation of atomic many-body dynamics is obtained, and time-interval averaged quantities can be directly solved. Since the conservation equations obtained by Chen and coworkers [2,3,5] are valid at the atomic scale, the field theory can reproduce time averaged atomic trajectories and can be used to investigate phenomena and properties that originated at the atomic scale. Since the field theory is formulated in terms of time-interval averaged quantities, it is expected to be computationally much more efficient than MD, and can be applied to simulate phenomena at both large length and time scales.

This paper is concerned with the application of the multiscale field theory. The primary goal of this work is to reproduce atomic scale properties and phenomena by the field theory. Atomistic formulation of the multiscale field theory is briefly introduced in Section 2, governing equations for problems with given temperature are derived in Section 3, simulations of dislocation nucleation and motion in a single crystal MgO under compression are presented in Section 4. We conclude this paper with a brief summary in Section 5.

2. Atomic formulation of a multiscale field theory

Microscopic dynamic quantities are functions of phase-space coordinates \((r,p)\), i.e., positions and momenta of atoms
\[
\begin{align*}
\mathbf{r} &= \{\mathbf{R}^{kz} = \mathbf{R}^k + \Delta \mathbf{r}^k\} \quad k = 1, 2, 3, \ldots n, \quad z = 1, 2, 3, \ldots v, \\
\mathbf{p} &= \{m^a \mathbf{V}^{kz} = m^a \mathbf{V}^k + m^a \Delta \mathbf{v}^k\} \\
& \quad k = 1, 2, 3, \ldots n, \quad z = 1, 2, 3, \ldots v,
\end{align*}
\]
where the superscript \(kz\) refers to the \(z\)th atom in the \(k\)th unit cell, \(m^a\) is the mass of \(a\)th atom, \(\mathbf{R}^{kz}\) and \(\mathbf{V}^{kz}\) are the position and velocity vector. \(\mathbf{R}^k\) and \(\mathbf{V}^k\) are the position and velocity of the center of the \(k\)th unit cell, respectively. The local density of any measurable phase-space function \(A(r,p)\) can generally be defined as
\[
A(x,y^k,t) = \sum_{k=1}^n \sum_{z=1}^v A(r(t),p(t)) \delta(\mathbf{R}^k - x) \delta(\Delta \mathbf{r}^k - y^z) \equiv A^k(x,t),
\]
with normalization conditions
\[
\int_p \delta(\mathbf{R}^k - x) \, d^3 x = 1 \quad (k = 1, 2, 3, \ldots n).
\]
Here, the first delta function is a localization function that provides the link between phase-space and physical space descriptions, it can be a Dirac \(\delta\)-function [15], or a distribution function [14]; \(V\) is the volume of the whole system. Eq. (2.3) implies that over the entire physical space all the unit cells, \((k = 1, 2, 3, \ldots n)\), can be found. Then, for each unit cell \(k\), the second \(\delta\)-function in Eq. (2.2), identifies \(y^z\) to be \(\Delta \mathbf{r}^k\), i.e.,
\[
\delta(\Delta \mathbf{r}^k - y^z) = \begin{cases} 
1 & \text{if } \Delta \mathbf{r}^k = y^z, \\
0 & \text{if } \Delta \mathbf{r}^k \neq y^z.
\end{cases}
\]

It follows
\[
\int_p \delta(\mathbf{R}^k - x) \delta(\Delta \mathbf{r}^k - y^z) \, d^3 x = 1 \quad (k = 1, 2, 3, \ldots n) \quad (z = 1, 2, \ldots v).
\]
Most current MD applications involve systems that are either in equilibrium or in some time-independent stationary state, where individual results are subject to fluctuation. It is the well-defined averages over sufficiently long time-intervals that are of interest. Extending MD to open systems, where coupling to the external world is more general, introduces many new problems. Not only are open systems out of thermodynamic equilibrium, but also in many cases they are spatially inhomogeneous and time-dependent. To smooth out the results and to obtain results close to experiments, measurements of physical quantities are necessary to be collected and averaged over finite time.
duration. Therefore, in deriving the field description of atomic quantities and balance equations, it is the time-interval averaged quantities that are used, and the time-interval averaged (at time \( t \) in the interval \( \Delta t \)) local density function takes the form

\[
\mathcal{T}(x, t) = \langle A' \rangle = \frac{1}{\Delta t} \int_0^{\Delta t} A'(x, t + \tau) d\tau
\]

\[
= \frac{1}{\Delta t} \int_0^{\Delta t} \sum_{k=1}^{n} A(r(t + \tau), p(t + \tau)) \times \delta(\mathbf{R}^k - x) \delta(\Delta k^x - y^x) d\tau.
\]  

(2.6)

The continuous local mass density \( \rho^z \), linear momentum density \( \rho^z(v + \Delta \mathbf{v}) \), internal energy density \( \rho^z \mathbf{u} \), temperature \( T^z \), internal force density \( f_{\text{int}}^z \) and external force density \( f^z \), are defined as

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

(2.7)

\[
\rho^z(v + \Delta \mathbf{v}) \equiv \left\langle \sum_{k=1}^{n} m^k (\mathbf{v}^k + \Delta \mathbf{v}^k) \delta(\mathbf{R}^k - x) \delta(\Delta k^x - y^x) \right\rangle,
\]

(2.8)

\[
\rho^z \mathbf{u} \equiv \left\langle \sum_{k=1}^{n} \left[ \frac{1}{2} m^k (\mathbf{v}^k \cdot \mathbf{v}^k + \mathbf{u}^k \cdot \mathbf{u}^k) \right] \delta(\mathbf{R}^k - x) \delta(\Delta k^x - y^x) \right\rangle,
\]

(2.9)

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

(2.10)

\[
f_{\text{int}}^z \equiv \left\langle \sum_{k=1}^{n} \left( \sum_{l=1}^{n} \sum_{\beta=1}^{v} f_{l}^\beta \mathbf{v}^k + \sum_{\beta=1}^{v} f_{2}^\beta \right) \delta(\mathbf{R}^k - x) \delta(\Delta k^x - y^x) \right\rangle,
\]

(2.11)

\[
\mathbf{f}^z \equiv \left\langle \sum_{k=1}^{n} f_{3}^\beta \delta(\mathbf{R}^k - x) \delta(\Delta k^x - y^x) \right\rangle.
\]

(2.12)

where, \( U^k \) is the potential energy, \( \frac{1}{2} m^k (\mathbf{v}^k)^2 + U^k = E^k \) is the atomic site energy of the \( k \)th atom in the \( k \)th unit cell; \( \mathbf{v}^k = \mathbf{v}^k + \Delta \mathbf{v}^k = \mathbf{v}^k + \Delta \mathbf{v}^k - \mathbf{v} - \Delta \mathbf{v}^k \) is the difference between the phase-space velocity and the local velocity field, \( k_B \) is Boltzmann constant; and \( \Delta V \) is the volume that defines the density of lattice points, i.e., the volume of a unit cell; \( f_{l}^\beta \) represents the interatomic force between \((k, z)\) and \((l, \beta)\) atoms in two different unit cells with \( f_{l}^\beta = -f_{l}^\beta; f_{l}^\beta \) the interatomic force between \((k, z)\) and \((k, \beta)\) atoms in the same unit cell with \( f_{l}^\beta = -f_{l}^\beta; f_{l}^\beta \) represents the body force on atom \((k, z)\) due to external fields.

The continuum counterpart of momentum flux density is the stress tensor. However, the mathematical infinitesimal volume that does not violate the continuum assumption in an atomistic system is the volume \( \Delta V \) defining the density of lattice points, which is the volume of a unit cell. The vector sum of all the atomic forces within this volume may not pass through the mass center of the \( \Delta V \). Therefore, the continuum stress is not the momentum flux density. For crystals with more than one atom in the unit cell, the continuum stress is only the homogeneous part of the momentum flux summing over a volume greater than or equal to that of a unit cell, and it may not be symmetric.

The total momentum flux is, therefore, better represented by decomposing it into a homogeneous part and an inhomogeneous part; each has a kinetic part and a potential part. The homogeneous part is caused by the lattice motion and deformation and is related to continuum stress. The inhomogeneous part is caused by internal (relative) atomic motion and deformation, and is the difference between the atomic momentum flux and classical definition of continuum stress. The homogeneous and inhomogeneous kinetic parts, \( \mathbf{f}_{\text{kin}} \) and \( \mathbf{v}_{\text{kin}} \), and the homogeneous and inhomogeneous potential parts, \( \mathbf{f}_{\text{pot}} \) and \( \mathbf{v}_{\text{pot}} \), take the following forms:

\[
\mathbf{f}_{\text{kin}} = -\left\langle \sum_{k=1}^{n} m^k \mathbf{v}^k \otimes \mathbf{v}^k \delta(\mathbf{R}^k - x) \delta(\Delta k^x - y^x) \right\rangle;
\]

(2.13)

\[
\mathbf{v}_{\text{kin}} = -\left\langle \sum_{k=1}^{n} m^k \Delta \mathbf{v}^k \otimes \mathbf{v}^k \delta(\mathbf{R}^k - x) \delta(\Delta k^x - y^x) \right\rangle;
\]

(2.14)

\[
\mathbf{f}_{\text{pot}} = -\left\langle \frac{1}{2} \int_0^1 d\lambda \sum_{k=1}^{n} \sum_{\zeta=1}^{v} \left( \mathbf{R}^k - \mathbf{R}^\lambda \right) \otimes f_{1}^\zeta \delta(\mathbf{R}^k \cdot \mathbf{R}^\lambda + \mathbf{R}^\lambda (1 - \lambda) - x) \delta(\Delta k^x \lambda + \Delta k^y (1 - \lambda) - y^x) \right\rangle;
\]

(2.15)

\[
\mathbf{v}_{\text{pot}} = -\left\langle \frac{1}{2} \int_0^1 d\lambda \sum_{k=1}^{n} \sum_{\zeta=1}^{v} \left( \Delta \mathbf{v}^k - \Delta \mathbf{v}^\lambda \right) \otimes f_{1}^\zeta \delta(\mathbf{R}^k \cdot \mathbf{R}^\lambda + \mathbf{R}^\lambda (1 - \lambda) - x) \delta(\Delta k^x \lambda + \Delta k^y (1 - \lambda) - y^x) \right\rangle - \left\langle \frac{1}{2} \int_0^1 d\zeta \sum_{k=1}^{n} \sum_{\zeta=1}^{v} \left( \Delta \mathbf{v}^k - \Delta \mathbf{v}^\lambda \right) \otimes f_{2}^\zeta \delta(\mathbf{R}^k - x) \delta(\Delta k^x \lambda + \Delta k^y (1 - \lambda) - y^x) \right\rangle.
\]

(2.16)
Similar to the decomposition of momentum flux density, the heat flux density is also decomposed into homogeneous and inhomogeneous kinetic parts, and homogeneous and inhomogeneous potential parts:

\[
q_{\text{kin}}^a = -\left( \sum_{k=1}^{a} \tilde{V}^k \left[ \frac{1}{2} m^x (\tilde{V}^k)^2 + U^{kx} \right] \delta(R^k - x) \delta(\Delta r^{kx} - y^x) \right); \\
\tilde{q}_{\text{kin}}^a = -\left( \sum_{k=1}^{a} \Delta \tilde{V}^k \left[ \frac{1}{2} m^x (\Delta \tilde{V}^k)^2 + U^{kx} \right] \delta(R^k - x) \delta(\Delta r^{kx} - y^x) \right); \\
q_{\text{pot}}^a = -\left( \frac{1}{2} \int_0^1 d\lambda \sum_{k,l=1}^{a} \sum_{\lambda=1}^{r} (R^k - R^l) \tilde{V}^{k\lambda} \cdot \tilde{f}_\lambda^a \delta(R^k \lambda + R^l (1 - \lambda) - x) \delta(\Delta r^{k\lambda} + \Delta r^{l0}(1 - \lambda) - y^x) \right); \\
\tilde{q}_{\text{pot}}^a = -\left( \frac{1}{2} \int_0^1 d\lambda \sum_{k,l=1}^{a} \sum_{\lambda=1}^{r} (\Delta r^{k\lambda} - \Delta r^{l0}) \tilde{V}^{k\lambda} \cdot \tilde{f}_\lambda^a \delta(R^k \lambda + R^l (1 - \lambda) - x) \delta(\Delta r^{k\lambda} + \Delta r^{l0}(1 - \lambda) - y^x) \right) - \left( \frac{1}{2} \int_0^1 d\lambda \sum_{k,l=1}^{a} \sum_{\lambda=1}^{r} (\Delta r^{k\lambda} - \Delta r^{l0}) \tilde{V}^{k\lambda} \cdot \tilde{f}_\lambda^a \delta(R^k - x) \delta(\Delta r^{k\lambda} + \Delta r^{l0}(1 - \lambda) - y^x) \right). \tag{2.20}
\]

It is noticed that the decomposition of fluxes actually is a consequence of the decomposition of atomic position into lattice position and relative atomic position. Amazingly, by decomposing atomic displacements, momentum and heat fluxes into homogeneous and inhomogeneous parts, the field representation of conservation laws at atomic scale can be formulated [2,3,5]. The mathematical representations of conservation equations for averaged mass, linear momentum and energy at atomic scale have been obtained as

\[
\frac{\partial \bar{\rho}^x}{\partial t} + \nabla_x \cdot (\bar{\rho}^x \bar{v}) + \nabla_y \cdot (\bar{\rho}^x \bar{a}) = 0, \tag{2.21}
\]

\[
\frac{\partial (\bar{\rho}^x (\bar{v} + \Delta \bar{v}))}{\partial t} = \nabla_x \cdot \left[ \tilde{f} - \bar{\rho}^x \bar{a} \otimes (\bar{v} + \Delta \bar{v}) \right] + \nabla_y \cdot \left[ \bar{\rho}^x \bar{a} \otimes \Delta \bar{v} \otimes (\bar{v} + \Delta \bar{v}) \right] + \tilde{f}^x, \tag{2.22}
\]

\[
\frac{\partial (\bar{\rho}^x \bar{e}^x)}{\partial t} + \nabla_x \cdot (\bar{q}^x + \bar{q} \bar{e}^x) + \nabla_y \cdot (-\tilde{J} - \bar{a} \Delta \bar{v} \bar{e}^x) = \bar{e}^x \cdot \nabla_x (\bar{v} + \Delta \bar{v}) + \tilde{e}^x \cdot \nabla_y (\bar{v} + \Delta \bar{v}). \tag{2.23}
\]

The atomic measure of the strains and the constitutive relations for the stresses (the homogeneous and the inhomogeneous parts, respectively) were obtained by Chen et al. [6]. Three strain measures were obtained as a result of the formulation. They are lattice deformation gradient, relative atomic deformation gradient and relative atomic-bond stretch/compression, with which atomic trajectories and atomic momentum flux can be fully reproduced. It was shown that the atomic stress is nonlinear and nonlocal in strains, involving an infinite series of higher order deformation gradients, and the 0th order stress is identical to the virial stress [6].

The field description of heat flux and internal energy were obtained by Chen et al. [7]. Similar to the momentum theorem [17] and is a function of temperature rate and strain rate.

Note that all the quantities in the balance Eqs. (2.21), (2.22), (2.23) are time-interval averaged quantities. This is one major difference between the field representation of the many-body dynamics and MD simulation: MD solves for instantaneous quantities first and then obtains averaged quantities through time averaging, while the field theory solves directly for averaged quantities, i.e., local thermal equilibrium properties, of which the fluctuations are averaged out. The procedure of taking time averages in MD or ensemble averages in statistical mechanics simulation is eliminated.

Another fundamental difference between MD and the field theory is that the lattice deformation is assumed to be continuous with respect to \(x\) in the field theory. This assumption requires that the smallest \(\Delta x\), e.g., the mesh size, should not be smaller than the lattice spacing. In the case of the finest mesh, \(\Delta x\) equals lattice spacing, and the field theory will have the same degrees of freedom as MD. However, since it is a field theory and is in terms of field variables such as displacement field and local densities, different meshes can be used in different regions for different concerns. This then enables the application of the field theory to systems with large length scales.

Also, since it is an atomic field theory and analytically links atomic and continuum descriptions of solid materials, it is naturally a concurrent atomic/continuum model. Both MD simulation and continuum modeling techniques can be utilized. As a result, the field-theory-based simulation shall be computationally much more efficient for statistical, finite size and finite temperature problems, for simultaneously large length and time scales phenomena, and especially, for dynamic and time-dependent systems.
3. Governing equations for problems with given temperature

Unlike many-body dynamics, a field theory is concerned with continuous local densities, such as mass density, momentum density, energy density, stress tensor, heat flux, etc. It is generally built upon two foundations: (1) the balance laws, and (2) the constitutive relations. With the balance laws and the constitutive relations, the dynamic behavior of a material system under a given external field and properly imposed boundary and initial conditions can be uniquely and completely determined in terms of a continuum description. Decomposing the atomic displacements into lattice and internal displacements, it is found that the stresses, internal energy, heat flux as well as the balance equations all can be expressed in terms of field variables [5–7], resulting in a well-posed boundary-value problem, in which the state or the independent variables are lattice displacement \( \mathbf{u}(\mathbf{x}) \), relative atomic displacements \( \zeta(\mathbf{x}, x) \) and temperature \( T^\delta, \alpha = 1, 2, \ldots, \nu \).

Temperature in most MD simulations is simply defined in terms of thermal energy by the mean-squared velocity relative to the local stream velocity. An important conceptual issue of temperature is the size of the region over which temperature is defined. For quantum mechanics definition, the length scale is defined by the mean-free-path of phonon. A local region with a designated temperature must be larger than the phonon scattering distance. This phonon viewpoint of temperature implies that the temperature cannot be defined for a particular atom, or a plane of atoms. The classical definition of temperature is entirely local, and one can define a temperature for each atom or a plane of atoms [1]. Here, we may just follow the classical way, and define a measure of thermal motion of atoms averaging over a unit cell and over a finite duration, and call it local temperature:

\[
T(\mathbf{x}) = \left( \frac{2\Delta V}{3k_B} \sum_{k=1}^{n} \sum_{s=1}^{1} \frac{1}{2} m^s (\mathbf{\bar{v}}^{ks})^2 \delta(\mathbf{R}^k - \mathbf{x}) \right). \tag{3.1}
\]

It is seen that the temperature can be further decomposed into a homogeneous part that is due to the motion of lattice, and an inhomogeneous part that is due to the atomic motion relative to the lattice as

\[
T(\mathbf{x}) = \left( \frac{2\Delta V}{3k_B} \sum_{k=1}^{n} \sum_{s=1}^{1} \frac{1}{2} m^s (\mathbf{\bar{v}}^k)^2 \delta(\mathbf{R}^k - \mathbf{x}) \right) + \left( \frac{2\Delta V}{3k_B} \sum_{k=1}^{n} \sum_{s=1}^{1} \frac{1}{2} m^s (\mathbf{\bar{v}}^{ks})^2 \delta(\mathbf{R}^k - \mathbf{x}) \right) = T_h + T_{ih}, \tag{3.2}
\]

where \( T_h \) and \( T_{ih} \) represent the homogeneous and inhomogeneous parts of temperature, respectively. These definitions may be useful when the homogeneous and inhomogeneous thermal stresses are of concern. From the phonon viewpoint of temperature, there may be excitations of acoustic phonons and optical phonons, and Eq. (3.2) may be viewed as a sum of thermal energy due to acoustic vibration modes and optical vibration modes. At temperature higher than Debye temperature, all modes have approximately the same energy [12]. It follows:

\[
T_h = \frac{1}{\nu} T, \tag{3.3}
\]
\[
T_{ih} = \frac{\nu - 1}{\nu} T, \tag{3.4}
\]

where \( \nu \) is the number of atoms per primitive unit cell.

Note that the kinetic stresses \( t \) and \( \tau \) are related to temperature as [6]

\[
t_{\text{kin}} = -\gamma_1 T^\delta \mathbf{I}, \tag{3.5}
\]
\[
\tau_{\text{kin}} = -\gamma_2 T^\delta \mathbf{I}, \tag{3.6}
\]

where \( \gamma_1 + \gamma_2 = \gamma \) and \( \gamma = k_B/\Delta V \). With Eqs. (3.3), (3.4), (3.5), (3.6), one has

\[
t_{\text{kin}} = -\frac{m^s}{M} \frac{k_B}{\Delta V} T \mathbf{I} \triangleq -\gamma k_B T \mathbf{I}/\Delta V, \tag{3.7}
\]
\[
\tau_{\text{kin}} = -(1 - \frac{m^s}{M}) k_B T \mathbf{I}/\Delta V \triangleq (1 - \gamma) k_B T \mathbf{I}/\Delta V. \tag{3.8}
\]

Here \( \gamma^d = m^d/M \), and \( M \equiv \sum_{\nu=1}^{d} m^\nu \) is the mass of the unit cell.

Now, rewrite the balance equation of linear momentum, Eq. (2.22), as

\[
\dot{\rho} \frac{d}{dt}(\mathbf{v} + \mathbf{\bar{v}}^o) = \nabla x \cdot \mathbf{t}^s + \nabla_{\mathbf{v}^o} \cdot \mathbf{\bar{t}}^d + \mathbf{\bar{f}}^o. \tag{3.9}
\]

With the relation between the momentum flux density and the internal force density [3]

\[
\nabla x \cdot \mathbf{f}_{\text{pot}} + \nabla_{\mathbf{v}^o} \cdot \mathbf{\bar{f}}_{\text{pot}} = \mathbf{f}_{\text{int}}^o, \tag{3.10}
\]

and with the relation between kinetic stress and temperature, Eqs. (3.7) and (3.8), one finds

\[
\dot{\rho} \frac{d}{dt}(\mathbf{v} + \mathbf{\bar{v}}^o) + \gamma k_B \Delta V \nabla x T = \mathbf{f}_{\text{int}}^o + \mathbf{f}^o. \tag{3.11}
\]

Now, if one has the constitutive relations for the internal force density \( \mathbf{f}_{\text{int}}^o \) as a function of the atomic positions or displacements at thermal equilibrium, which can be obtained through fitting to quantum mechanics calculations, then for systems with given temperature, i.e., homogeneous temperature field or a steady state temperature field with a constant temperature gradient, Eq. (3.11) together with Eq. (2.21) can serve as the governing equations for time-interval averaged atomic displacements. For crystalline materials below half of the melting temperature, one may assume the mass density remains constant during deformation, then Eq. (3.11) alone can serve as the governing equation, i.e.,

\[
\dot{\rho} \mathbf{u}(\mathbf{x}) + \gamma k_B \Delta V \nabla x T^o(\mathbf{x}) = \mathbf{f}_{\text{int}}^o(\mathbf{x}) + \mathbf{f}^o, \tag{3.12}
\]
where \( \mathbf{u}_0 = \mathbf{u}(t) \) is a specified displacement function of time; the superscript \( A \) refers to all the atoms in the top and bottom loading zones (zone A as shown in Fig. 2c); the \( \mp \) sign indicates a compressive loading. Three loading cases have been considered in this paper. The specified displacement function for each case is shown in Fig. 3. Also, for all the three

\[
\begin{align*}
\mathbf{f}_{\text{int}}^a &= \int_{\Omega(x)} \sum_{\beta=1}^n f(\mathbf{u}^a(x) - \mathbf{u}^a(x')) \, d\mathbf{x}' , \quad (3.12) \\
\mathbf{u}^a(x) &= \mathbf{u}(x) + \mathbf{\xi}(x,z), \quad (3.13) \\
\mathbf{u}(x) &= \frac{1}{M} \sum_{z=1}^s m^z \mathbf{u}^z. \quad (3.14)
\end{align*}
\]

Note that the constitutive relation for the interatomic force density \( \mathbf{f}_{\text{int}}^a \) can also be derived from the instantaneous analytical interatomic force–displacement relation. For crystalline materials below half melting temperature, one can show that the functional relationship between the averaged atomic force and the atomic positions at thermal equilibrium can be approximated to the instantaneous counterpart, i.e., \( \mathbf{f}(\mathbf{r}) \approx \mathbf{f}'(\mathbf{r}) \), where \( \mathbf{r} \) is the atomic positions at thermal equilibrium. It is emphasized that for thermal-mechanical coupling problems, e.g., situations where local temperature can be generated by plastic deformations, then Eqs. (2.21), (2.22), (2.23) are needed to solve for the atomic displacements and local temperature.

### 4. Modeling and simulation of MgO under compression

\( \text{MgO} \) is a material of significant scientific and engineering importance. At ambient conditions it has the rocksalt structure with lattice constants \( a = b = c = 4.2 \) Å (cf. Fig. 1), and has the peculiarity of not showing any phase transition at least up to 227 GPa. A fundamental understanding of its mechanical properties is a prerequisite for the correct description of more complex oxides or silicates. The comparative simplicity of MgO with respect to other minerals means that it has become the standard test-bed for the evaluation of theoretical methods.

In this work, a nanoscale single crystal MgO specimen subject to compressive loading is modeled by the field theory [referred as Multiscale Modeling (MM)]. The specimen consists of \( 7 \times 7 \times 7 \) unit cells with eight atoms per unit cell. A displacement controlled loading is applied. The loading process is divided into two stages: (1) a loading stage in which the displacement is linearly increasing with time, and (2) a holding stage in which the enforced displacement is held as constant in time. The loading condition may be expressed as

\[
u^i_0 = 0, \quad \nu^i_2 = \mp \mathbf{u}(t), \quad (4.1)
\]

where \( \mathbf{u}(t) \) is a specified displacement function of time; the superscript \( A \) refers to all the atoms in the top and bottom loading zones (zone A as shown in Fig. 2c); the \( \mp \) sign indicates a compressive loading. Three loading cases have been considered in this paper. The specified displacement function for each case is shown in Fig. 3. Also, for all the three

![Fig. 1. Crystal structure of MgO.](image)

![Fig. 2. Computational model: (a) the lattice, (b) the atomic arrangement and (c) boundary conditions.](image)

![Fig. 3. Loading conditions.](image)

<table>
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<th>Species</th>
<th>Species</th>
<th>( A ) (eV)</th>
<th>( \rho ) (Å)</th>
<th>( C' ) (eV Å(^6))</th>
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</tbody>
</table>

Table 1: Short-range interaction parameters for different pairs in magnesia.
cases in this work, we used a homogeneous temperature field of $T = 300$ K for the purpose of comparison with MD simulation results.

The combination of Coulomb and Buckingham potentials is employed to specify the atomic interaction:

$$U(r_{ij}) = \frac{z_i z_j e^2}{r_{ij}} + A_{ij} e^{-r_{ij}/\rho} - \frac{C_{ij}}{r_{ij}^6},$$

(4.2)

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ is the separate distance between the two atoms; the first term in Eq. (4.2) is the long-range Coulomb potential energy where $z_i$ and $z_j$ are the charges of “$i$ ion” and “$j$ ion”; the second term is the repulsive or overlap energy approximated by the Born–Mayer potential; the last term is the van der Waals attractive energy which represents the correlated motions of electrons on different ions as a dipole-induced dipole interaction where parameters

Fig. 4. Averaged stresses of the specimen for three loading cases.

Fig. 5. Stress distribution and its time evolution for Case-1 (side view).

Fig. 6. Crystal structural evolution over time for Case-1 (side view).

Fig. 7. Stress distribution and its time evolution for Case-3 (side view).

Fig. 8. Crystal structural evolution over time for Case-3 (side view).
\( q \), \( A_{ij} \) and \( C_{ij} \), as shown in Table 1, were obtained by Grimes [13] through fitting to experimental results.

The averaged stresses \( \sigma_{zz} \) obtained in all the three cases are plotted in Fig. 4. It is seen that in the smallest loading case (Case-1), the stress increases linearly with time, i.e., with applied displacement, in the loading stage, and remains constant at the holding stage. For each of the two larger loading cases, a sudden drop in the averaged stress was observed before the end of loading stage and afterwards the stress oscillates with time. It takes a longer
time for the oscillations to vanish in the largest loading case (Case-3) than that in the smaller loading case (Case-2).

Fig. 5 is the time evolution of stress $\sigma_{zz}$ distribution in Case-1. Fig. 6 presents the side views of the structural evolution of the crystal. It is seen that, as loading increases, a compressive stress develops, but the crystal remains stable and perfect during both the loading and holding stages. The specimen is in a state of elastic deformation.

Fig. 7 is the time evolution of the stress distribution in Case-3. Fig. 8 is the corresponding side views of the atomic arrangement. It is seen that there exists a maximum compressive stress (indicated by blue color in Fig. 7) at time equals to 0.72 ps. When all the points in the entire specimen reach this critical stress, the material loses its stability, it yields, and a tensile stress develops (indicated by red color in Fig. 7). It is shown from Fig. 8 that, corresponding to the critical stress point, dislocations initiate. This explains the sudden drop in the averaged stress curve (cf. Fig. 4) as a result of the development of tensile stress (cf. Fig. 7) or as a consequence of dislocation nucleation (Fig. 8).

Fig. 9 (side views) and Fig. 10 (top views) provide further information on the structural evolution in Case-3 during the loading stage and the holding stage. It is interesting to see, at the holding stage, while the loading remains constant, the atoms continue to move. As a result of the motion of the dislocations, the stress oscillates until all the dislocations move out of the specimen (cf. Fig. 10). We see that steps have been formed, permanent plastic deformations have been generated (cf. Fig. 10), and amazingly, the crystal structure becomes ordered again during the holding stage (cf. Figs. 9 and 10).

Fig. 11 is a comparison between the averaged stress by the field theory (MM) and that by MD. The MD results are obtained by DL-POLY, a general-purpose parallel MD simulation code [16], and the Hoover constant temperature algorithm (NVT) is employed in all the MD simulations with a constant temperature field $T = 300$ K. It is seen that the results of stress curves in these two independent simulations are in good agreement. However, it is seen that in Case-1, the elastic case, the averaged stress at holding stage from MD oscillates over time, while that obtained by MM is almost flat. This is because, while MD solves and outputs instantaneous quantities, MM solves and outputs time-interval averaged quantities of which thermal fluctuations are averaged out. It is seen that for the largest loading case (Case-3), beyond the critical stress point, the averaged stress by MM oscillates, but the oscillations disappear in time as the enforced constant displacement continue to hold. 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 with time is the consequence of the motion of dislocations, since in the two larger loading cases (Case-2 and Case-3), the oscillations vanish when all the dislocations have moved out of the specimen, and it takes longer time for the oscillations to vanish in the larger loading case (Case-3) than that in the relative smaller loading case (Case-2).

5. Summary and discussion

This paper summarizes an atomistic formulation of a multiscale field theory, and presents the simulation results of MgO under compression by the theory. A critical stress for MgO under compression is obtained, which is found to be independent of the magnitude of loading. Corresponding to the critical stress point, dislocation initiates, thus explaining the sudden drop in the averaged stress curve as a result of the development of local tensile stress or as a consequence of dislocation nucleation.

It is interesting to see, while the applied loading remains constant, the atoms continue to move. As a result of the motion of dislocations, the stress oscillates until all dislocations move out of the crystal. We see that steps have been formed, permanent plastic deformations have been

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*Fig. 11. A comparison of the averaged stress of the specimen by MM and by MD: (a) Case-1 and (b) Case-3.*
generated, and amazingly, the material becomes ordered again while there is still a constant applied load. It should be emphasized that all of these were found within ionic materials at nanometer in length and picosecond in time. Thus, this simulation also confirms that dislocation velocity is comparable with sound velocity [9].

The well known microcontinuum theories and/or generalized continuum theories, such as Micromorphic theory [10], Microstructural theory [11] and Cosserat theory [8], view a material as a continuum with microstructure. They are the extensions of classical continuum mechanics to the application at small length scales. They admit that the stress may not be symmetric at small length scales and thus introduce the additional and higher order stresses such as couple stress or moment stress as well as additional internal variables to describe the effect of the inhomogeneous motion and deformation. Note that those theories assume the smallest structural unit of a material (e.g., the primitive unit cell for a single crystal) as a continuum. As a consequence, those continuum theories are not applicable to phenomena that take place at length scale smaller than a unit cell. Compared with microcontinuum theories, this newly formulated field theory extends the application of a continuum field theory to the atomic scale.

Dislocation nucleation and motion is a phenomenon that takes place at atomic length and time scale. From the simulation of MgO under compression in this paper, we see that the field theory can model and simulate critical phenomena that take place at atomic length/time scale. While the numerical implementation of this field theory is still an ongoing work, the present simulation has shown us that atomic scale material behavior, elastic properties and yielding behavior of materials can be reasonably reproduced by the field theory. Comparing the results obtained by the field theory with that by MD, we find that it is the time averaged properties and time averaged atomic trajectories that are solved and output by the field theory as opposed to the instantaneous properties and instantaneous atomic positions that are solved and output in MD simulations. Thus, we believe that the field theory may not only provide an analytical and computational link between atomistic models and continuum field theory, but can also serve as a multiscale material modeling tool for concurrent atomic/continuum modeling and simulations.

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References