

Journal of
***Mechanics of
Materials and Structures***

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SCALES**

Youping Chen, James Lee and Liming Xiong

Volume 1, N° 4

April 2006

 mathematical sciences publishers

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YOUPIING CHEN, JAMES LEE AND LIMING XIONG

This paper is concerned with stress and strain fields at atomic scale. Unlike other formulations of atomistic expression of macroscopic stress fields or homogeneous systems, this paper aims at field descriptions of atomic stresses and strains for multi-element crystalline materials. By decomposing atomic deformation into homogeneous lattice deformation and inhomogeneous relative atomic deformation, a field representation of momentum flux is formulated within the framework of atomic many-body dynamics, and the connection to a macroscopic definition of stress is obtained. The atomic strain measures and the atomic stress-strain relations are derived. Phonon dispersion relations are calculated and presented.

1. Introduction

Stress is an important concept in characterizing the states of condensed matter, and has been extensively studied from both macroscopic and microscopic points of view. Quantum mechanics theory of stress may be traced back to the earliest years of the development of quantum mechanics [Born et al. 1926]. Through atomistic simulations of momentum flux in classical many-body dynamics, the study of stress response to external disturbance has played an important role in understanding mechanical properties of materials [Horstemeyer and Baskes 1999]. One of the fundamental properties in classical continuum mechanics is stress. Extensions of macroscopic continuum theory to microcontinuum theories are mainly due to the deficiency of stress descriptions – we thus have theories incorporating moment stress, microstress average, couple stress, etc. [Eringen and Suhubi 1964; Mindlin 1964; Eringen 1967; Cosserat and Cosserat 1909; Toupin 1962; Green and Rivlin 1964]. While the underlying physics is same, the descriptions from different viewpoints are thoroughly different.

Atomistic view of a crystal is as a periodic arrangement of local atomic bonding units. Each lattice point defines the location of the center of the unit that forms the smallest structural unit of the crystal. The structure of the unit together with

Keywords: stress, strain, atomic scale, many-body dynamics.

The support to this work by National Science Foundation under Award Numbers CMS-0301539 and CMS-0428419 is gratefully acknowledged.

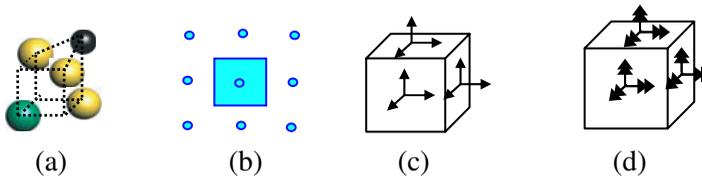


Figure 1. Stresses in ABO_3 ferroelectrics: (a) The ABO_3 structural unit; (b) Lattice points and the unit cell (2D illustration); (c) stress evaluated at lattice position with the volume of a unit cell; (d) moment stress resulting from the resultant moment of interatomic forces.

the network of lattice points determines the crystal structure and hence the physical properties of the material. Classical continuum mechanics, on the other hand, views a crystal as a homogeneous and continuous medium. The basic structural unit of the crystal is idealized as point mass, and the internal motion and deformation of atoms within the unit are ignored.

Consider ABO_3 ferroelectrics as an example. There are five atoms in a unit cell, the smallest structural unit (Figure 1a). This unit cell (a mass point in classical continuum theory) gives the smallest allowable volume in which the continuum hypothesis is not violated (Figure 1b). However, at ferroelectric phase, for this mathematical infinitesimal, the vector sum of all interatomic forces will not pass through the mass center. This will result in a surface couple on the surface of this infinitesimal volume, and hence a higher order moment stress, \mathbf{m} , (as shown in Figure 1d) in addition to the stress in the traditional continuum definition (Figure 1c). Such higher order stress has been employed in many micro-continuum theories to account for the effect of microstructure. Among those well-established, there are micromorphic theory [Eringen and Suhubi 1964; Eringen 1999], microstructure theory [Mindlin 1964], micropolar theory [Eringen 1967], and Cosserat theory [Cosserat and Cosserat 1909]. As a consequence of the higher order stresses, there are higher order strains to be the corresponding thermodynamic conjugates.

However, it is very difficult, if not impossible, for these micro-continuum theories to describe the dynamics feature of atoms in complex crystals at nano/micro scales. Material properties or behavior related to atomic motion and interaction cannot be modeled accurately by the existing micro-continuum theories. Moreover, the stresses and strains defined in classical or micro-continuum theories may not be consistent with the atomistic definitions in microscopic modeling and simulations.

This paper aims at field descriptions of stress and strain at atomic scale for multi-element crystals. In Section 2 the momentum flux density in the classical N -body dynamics will be introduced. A field representation of momentum flux will be derived in Section 3, atomic stress-strain relation as well as the atomistic measures

of strain will be derived in Section 4, a few numerical examples will be presented in Section 5, and a summary and discussions will be presented in Section 6. Standard dyadic and tensor notations are employed in this paper.

2. Momentum flux in classical N -body dynamics

2.1. Atomic forces. In an atomic N -body system, if one defines the force between atom i and atom j as

$$\mathbf{f}^{ij} = - \left\langle \frac{\partial U_{\text{int}}}{\partial (\mathbf{R}^i - \mathbf{R}^j)} \right\rangle = \left\langle \frac{\partial U_{\text{int}}}{\partial (\mathbf{R}^j - \mathbf{R}^i)} \right\rangle = - \mathbf{f}^{ji}, \quad (2-1)$$

one then has

$$\mathbf{f}^i = \sum_{j=1}^n \mathbf{f}^{ij},$$

where \mathbf{f}^{ij} is the interatomic force and $\mathbf{R}^i - \mathbf{R}^j$ the relative separation vector between the two atoms i and j .

Now consider a multi-element crystal with n unit cell and ν atoms in each primitive unit cell. Generally, forces acting on an atom (k, α) , where $k = 1, 2, \dots, n$ and $\alpha = 1, 2, \dots, \nu$, can be divided into three kinds:

1. $\mathbf{f}_1^{k\alpha}$: interatomic force between (k, α) and (l, β) atoms in two different unit cells k and l , with

$$\mathbf{f}_1^{l\beta} = - \mathbf{f}_1^{k\alpha}.$$

2. $\mathbf{f}_2^{k\alpha}$: interatomic force between (k, α) and (k, β) atoms in the same unit cell k , with

$$\mathbf{f}_2^{k\alpha} = - \mathbf{f}_2^{k\beta}.$$

3. $\mathbf{f}_3^{k\alpha}$: body force on atom (k, α) due to the external fields.

The total force acting on an atom (k, α) can be written as

$$\mathbf{F}^{k\alpha} = \sum_{l=1}^n \sum_{\beta=1}^{\nu} \mathbf{f}_1^{l\beta} + \sum_{\beta=1}^{\nu} \mathbf{f}_2^{k\beta} + \mathbf{f}_3^{k\alpha}.$$

2.2. Momentum flux. The quantum mechanical theorem of stress by Born et al. [1926] and Nielsen and Martin [1985] can result in exactly the same form as the momentum flux in classical many-body dynamics [Hoover 1986; 1991; Chen and Lee 2003a; 2003b]. On a microscopic basis of atomic many-body dynamics, there are two kinds of contributions to the momentum flux: kinetic and potential.

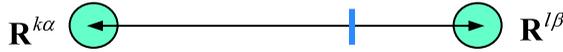


Figure 2. Flow of momentum due to inter-particle force.

Suppose a particle α carries a momentum \mathbf{p} . During a small time interval dt this momentum is transported a distance $(\mathbf{p}/m^\alpha)dt$. The resulting “kinetic” contribution to the momentum flux, in the co-moving coordinate system, is

$$\mathbf{s}_{\text{kin}}^\alpha = -\mathbf{p} \otimes \mathbf{p}/m^\alpha. \quad (2-2)$$

By virtue of the possible macroscopic motion of the material body, the velocity that contributes to momentum flux is the difference between the instantaneous velocity and the stream velocity (the ensemble or time-interval average of the velocity),

$$\tilde{\mathbf{V}}^{k\alpha} = \mathbf{V}^{k\alpha} - \langle \mathbf{V}^{k\alpha} \rangle = \mathbf{V}^{k\alpha} - (\bar{\mathbf{v}} + \Delta\bar{\mathbf{v}}^\alpha). \quad (2-3)$$

This velocity difference, $\tilde{\mathbf{V}}^{k\alpha}$, measures the fluctuations of atoms relative to the local equilibrium and is related to the thermal motion of atoms.

The “potential” flow of momentum occurs through the mechanism of the inter-particle forces. For a pair of particles $k\alpha$ and $l\beta$ that lie on different sides of a surface, the pair force

$$\mathbf{f}^{l\beta}{}^{k\alpha} = -\mathbf{f}^{k\alpha}{}^{l\beta}$$

gives the rate at which momentum is transported from particle $k\alpha$ to particle $l\beta$. For each such pair the direction of this transport is along the line parallel to $\mathbf{R}^{k\alpha} - \mathbf{R}^{l\beta}$, and the potential contribution to the momentum flux is

$$\mathbf{s}_{\text{pot}} = -\mathbf{R}^{k\alpha} \otimes \mathbf{f}^{l\beta}{}^{k\alpha} - \mathbf{R}^{l\beta} \otimes \mathbf{f}^{k\alpha}{}^{l\beta} = -(\mathbf{R}^{k\alpha} - \mathbf{R}^{l\beta}) \otimes \mathbf{f}^{l\beta}{}^{k\alpha}. \quad (2-4)$$

This momentum transfer can be visualized as a direct connection between two interacting particles (Figure 2), which is continuous through the line linking them.

3. Field representation of momentum flux

3.1. Field representation of the atomic system. An ordered atomic system can be viewed as a periodic arrangement of local atomic bonding units. Each lattice point defines the location of the center of the unit. The space lattice is macroscopically homogeneous, and the deformation of lattice is homogeneous up to the point of structural instability (phase transformation). Therefore, the network of lattice point is continuous, and the deformation gives rise to a field function $\mathbf{u}(\mathbf{x})$, where each point \mathbf{x} in the physical space corresponds to a lattice point \mathbf{R}^k in the phase space;

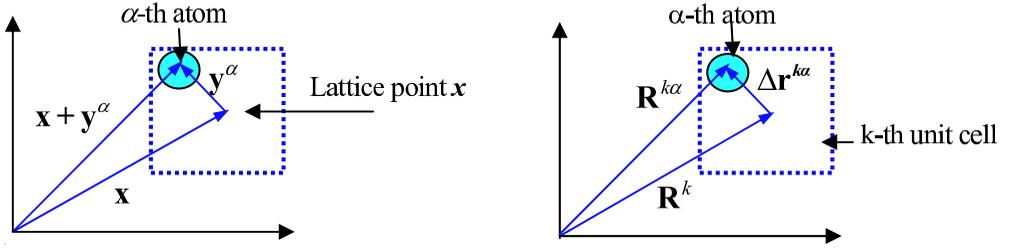


Figure 3. Physical space and phase space descriptions of an atomic position.

embedded within each point \mathbf{x} is a group of ν discrete atoms ($\Delta \mathbf{r}^{k\alpha}$) (Figure 3). With a localization function

$$\delta(\mathbf{R}^k + \Delta \mathbf{r}^{k\alpha} - \mathbf{x} - \mathbf{y}^\alpha) = \delta(\mathbf{R}^k - \mathbf{x})\delta(\Delta \mathbf{r}^{k\alpha} - \mathbf{y}^\alpha),$$

the local density of any measurable phase-space function $A(\mathbf{r}, \mathbf{p})$, where

$$A(\mathbf{r}, \mathbf{p}) = A(\mathbf{r}(t), \mathbf{p}(t)),$$

can be expressed as [Chen and Lee 2006]

$$\bar{A}^\alpha(\mathbf{x}, t) = \langle A^\alpha \rangle \equiv A_m^\alpha = \frac{1}{\Delta t} \int_0^{\Delta t} \sum_{k=1}^n A(\mathbf{r}, \mathbf{p}) \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\alpha} - \mathbf{y}^\alpha) d\tau,$$

Here, quantities in physical space are expressed in terms of time-interval averages, as in experimental observations, which are performed over a finite duration. The localization function, a Dirac δ -function or a distribution function, links the expressions of a dynamic function in phase space to the local density function in physical space. The displacement of lattice point \mathbf{x} , $\mathbf{u}(\mathbf{x})$, gives rise to the homogeneous and continuous lattice deformation with length scale from nano to macroscopic. The relative displacements of the α -th atom, $\xi(\mathbf{x}, \alpha)$, result in relative atomic deformation within the inner structure and describe the inhomogeneous and non-continuum atomic behavior whose length scale is less than a nanometer. The total atomic displacement is $\mathbf{u}(\mathbf{x}) + \xi(\mathbf{x}, \alpha)$ in physical space, corresponding to the $\mathbf{u}(k) + \xi(k, \alpha)$ in phase space, with the time scale of $\mathbf{u}(\mathbf{x})$ at audible frequency region and $\xi(\mathbf{x}, \alpha)$ at inferred.

3.2. Field descriptions of forces and momentum flux. The field representation of total force acting on an atom α can be expressed as

$$\mathbf{F}^\alpha(\mathbf{x}) \equiv \left\langle \sum_{k=1}^n \left(\sum_{l=1}^n \sum_{\beta=1}^{\nu} \mathbf{f}_1^{l\beta k\alpha} + \sum_{\beta=1}^{\nu} \mathbf{f}_2^{k\beta} + \mathbf{f}_3^{k\alpha} \right) \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\alpha} - \mathbf{y}^\alpha) \right\rangle,$$

where the external body force density $\bar{\mathbf{f}}^\alpha$ is given by

$$\bar{\mathbf{f}}^\alpha(\mathbf{x}) \equiv \left\langle \sum_{k=1}^n \mathbf{f}_3^{k\alpha} \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\alpha} - \mathbf{y}^\alpha) \right\rangle,$$

and the internal force density is (see Equation (2-1))

$$\bar{\mathbf{f}}_{\text{int}}^\alpha(\mathbf{x}) = \left\langle \sum_{k=1}^n \left(\sum_{l=1}^n \sum_{\xi, \eta=1}^v \mathbf{f}_1^{l\eta}{}^{k\xi} + \sum_{\xi, \eta=1}^v \mathbf{f}_2^{k\xi} \right) \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha) \right\rangle.$$

From Equations (2-2)–(2-4), the local densities of kinetic and potential momentum fluxes can be expressed as

$$\begin{aligned} \bar{\mathbf{s}}_{\text{kin}}^\alpha(\mathbf{x}) &= - \left\langle \sum_{k=1}^n m^\alpha \tilde{\mathbf{V}}^{k\alpha} \otimes \tilde{\mathbf{V}}^{k\alpha} \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\alpha} - \mathbf{y}^\alpha) \right\rangle, \\ \bar{\mathbf{s}}_{\text{pot}}^\alpha(\mathbf{x}) &= - \left\langle \frac{1}{2} \sum_{k,l=1}^n \sum_{\xi, \eta=1}^v (\mathbf{R}^{k\xi} - \mathbf{R}^{l\eta}) \right. \\ &\quad \left. \otimes \mathbf{f}_1^{l\beta}{}^{k\xi} \int_0^1 d\lambda \delta(\mathbf{R}^k \lambda + \mathbf{R}^l (1-\lambda) - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} \lambda + \Delta \mathbf{r}^{l\eta} (1-\lambda) - \mathbf{y}^\alpha) \right\rangle \\ &\quad - \left\langle \frac{1}{2} \sum_{k=1}^n \sum_{\xi, \eta=1}^v (\mathbf{R}^{k\xi} - \mathbf{R}^{k\eta}) \right. \\ &\quad \left. \otimes \mathbf{f}_2^{k\eta}{}^{k\xi} \int_0^1 d\lambda \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} \lambda + \Delta \mathbf{r}^{k\eta} (1-\lambda) - \mathbf{y}^\alpha) \right\rangle. \end{aligned}$$

The momentum flux in MD has been considered as the atomistic counterpart of the continuum stress. However, it is seen that

- (1) The smallest mathematical infinitesimal volume that does not violate the continuum assumption is the volume ΔV defining the density of lattice points, which is the volume of a primitive unit cell. The vector sum of all the atomic forces within this volume may not pass through the mass center of the ΔV (Figure 4).
- (2) The continuum definition of stress is not the momentum flux density. For a crystal with more than one atom in the unit cell, the continuum stress is only the homogenous part of the momentum flux summing over a volume of at least a primitive unit cell, and it may not be symmetric.

The total momentum flux density is, therefore, better represented by the sum of a homogeneous part, \mathbf{t} , which is due to the motion and deformation of the lattice

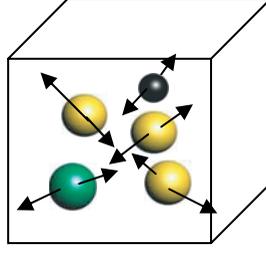


Figure 4. Illustration of atomic forces in a unit cell.

and is related to continuum stress,

$$\bar{\mathbf{i}}_{\text{kin}}^{\alpha} = - \left\langle \sum_{k=1}^n m^{\alpha} \tilde{\mathbf{V}}^k \otimes \tilde{\mathbf{V}}^{k\alpha} \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\alpha} - \mathbf{y}^{\alpha}) \right\rangle, \quad (3-1)$$

$$\bar{\mathbf{i}}_{\text{pot}}^{\alpha} = - \left\langle \frac{1}{2} \int_0^1 d\lambda \sum_{k,l=1}^n \sum_{\xi,\eta=1}^v (\mathbf{R}^k - \mathbf{R}^l) \otimes \mathbf{f}_1^{l\eta} \delta(\mathbf{R}^k \lambda + \mathbf{R}^l (1-\lambda) - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} \lambda + \Delta \mathbf{r}^{l\eta} (1-\lambda) - \mathbf{y}^{\alpha}) \right\rangle, \quad (3-2)$$

and an inhomogeneous part, τ , which is due to the internal motion and deformation,

$$\bar{\tau}_{\text{kin}}^{\alpha} = - \left\langle \sum_{k=1}^n m^{\alpha} \Delta \tilde{\mathbf{v}}^{k\alpha} \otimes \tilde{\mathbf{V}}^{k\alpha} \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\alpha} - \mathbf{y}^{\alpha}) \right\rangle, \quad (3-3)$$

$$\begin{aligned} \bar{\tau}_{\text{pot}}^{\alpha} = & - \left\langle \frac{1}{2} \int_0^1 d\lambda \sum_{k,l=1}^n \sum_{\xi,\eta=1}^v (\Delta \mathbf{r}^{k\xi} - \Delta \mathbf{r}^{l\eta}) \otimes \mathbf{f}_1^{l\beta} \delta(\mathbf{R}^k \lambda + \mathbf{R}^l (1-\lambda) - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} \lambda + \Delta \mathbf{r}^{l\eta} (1-\lambda) - \mathbf{y}^{\alpha}) \right\rangle \\ & - \left\langle \frac{1}{2} \int_0^1 d\lambda \sum_{k=1}^n \sum_{\xi,\eta=1}^v (\Delta \mathbf{r}^{k\xi} - \Delta \mathbf{r}^{k\eta}) \otimes \mathbf{f}_2^{k\eta} \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} \lambda + \Delta \mathbf{r}^{k\eta} (1-\lambda) - \mathbf{y}^{\alpha}) \right\rangle. \end{aligned} \quad (3-4)$$

Using the identity

$$\begin{aligned} & \frac{d}{d\lambda} \left(\delta(\mathbf{R}^k \lambda + \mathbf{R}^l (1 - \lambda) - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} \lambda + \Delta \mathbf{r}^{l\eta} (1 - \lambda) - \mathbf{y}^\alpha) \right) \\ &= -\nabla_{\mathbf{x}} \cdot \left((\mathbf{R}^k - \mathbf{R}^l) \delta(\mathbf{R}^k \lambda + \mathbf{R}^l (1 - \lambda) - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} \lambda + \Delta \mathbf{r}^{l\eta} (1 - \lambda) - \mathbf{y}^\alpha) \right) \\ & - \nabla_{\mathbf{y}^\alpha} \cdot \left((\Delta \mathbf{r}^{k\xi} - \Delta \mathbf{r}^{l\eta}) \delta(\mathbf{R}^k \lambda + \mathbf{R}^l (1 - \lambda) - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} \lambda + \Delta \mathbf{r}^{l\eta} (1 - \lambda) - \mathbf{y}^\alpha) \right), \end{aligned}$$

the divergences of the potential momentum fluxes can be related to the interatomic forces as

$$\begin{aligned} \nabla_{\mathbf{x}} \cdot \bar{\mathbf{t}}_{\text{pot}}^\alpha + \nabla_{\mathbf{y}^\alpha} \cdot \bar{\mathbf{t}}_{\text{pot}}^\alpha &= \mathbf{f}_{\text{pot}}^\alpha(\mathbf{x}) \\ &= \left\langle \sum_{k=1}^n \sum_{\eta=1}^v \left(\sum_{l=1}^n \mathbf{f}_1^{l\eta k\alpha} + \mathbf{f}_2^{k\eta} \right) \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\alpha} - \mathbf{y}^\alpha) \right\rangle. \end{aligned} \quad (3-5)$$

Note that for cell average $\bar{\mathbf{t}}_{\text{pot}}^\alpha = \sum_{\alpha=1}^v \bar{\mathbf{t}}_{\text{pot}}^\alpha$. Using $\sum_{\alpha,\beta=1}^v \mathbf{f}_2^{k\alpha\beta} = 0$, one finds

$$\nabla_{\mathbf{x}} \cdot \bar{\mathbf{t}}_{\text{pot}}^\alpha = \left\langle \sum_{k,l=1}^n \sum_{\alpha,\beta=1}^v \mathbf{f}_1^{l\beta k\alpha} \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \quad (3-6)$$

$$= \left\langle \sum_{k=1}^n \sum_{\alpha,\beta=1}^v \left(\sum_{l=1}^n \mathbf{f}_1^{l\beta k\alpha} + \mathbf{f}_2^{k\alpha\beta} \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle. \quad (3-7)$$

This is the well-known stress-force relation in the continuum description.

It is seen from Equations (3-5) and (3-6) that

$$\sum_{\alpha=1}^v \nabla_{\mathbf{y}^\alpha} \cdot \bar{\mathbf{t}}_{\text{pot}}^\alpha = 0.$$

This indicates that the divergence of the inhomogeneous momentum flux density will be averaged out and will not contribute to cell-averaged balance equation of linear momentum. However, note that

$$\sum_{\alpha=1}^v \bar{\mathbf{t}}_{\text{pot}}^\alpha \neq 0.$$

The inhomogeneous part of momentum flux does not vanish upon cell averaging. Therefore, as pointed out by Nielsen and Martin [1985], the classical definition of macroscopic stress as “any tensor field which satisfies the condition that its divergence is the vector force field” [Sommerfeld 1950; Nye 1957] cannot give a unique definition of stress, and additional consideration is required to include the

inhomogeneous part of momentum flux in order to uniquely describe the stress field at microscopic scale for inhomogeneous systems.

4. Stress-strain relations in the nano/micro scales

4.1. Interatomic forces. Results of atomic-level molecular dynamics simulation depend critically on the interatomic forces. A key issue in atomic-level simulations is therefore the choice of a suitable potential energy function or interatomic force. For the sake of simplicity, this paper considers only systems with central force pair potential. Assuming the separation distance of two atoms is d^{ij} , and the total potential energy of the system U is a function of the atomic positions only, one has

$$U = \sum_{i \neq j}^n U(d^{ij}).$$

Setting

$$G(d^{ij}) \equiv \frac{1}{d^{ij}} \frac{\partial U}{\partial (d^{ij})},$$

the interatomic force between atoms i and j can be written as

$$\mathbf{f}^{ij} = - \frac{\partial U}{\partial (\mathbf{d}^{ij})} = - \frac{\partial U}{\partial (d^{ij})} \frac{\mathbf{d}^{ij}}{d^{ij}} = - G(d^{ij}) \mathbf{d}^{ij}.$$

Here \mathbf{d}^{ij} is the separation vector between two atoms i and j .

In our notation the vectorial relative displacement between atom (k, α) and atom (l, β) is

$$\mathbf{R}^{k\alpha} - \mathbf{R}^{l\beta} = (\mathbf{R}_o^{k\alpha} - \mathbf{R}_o^{l\beta}) + \mathbf{u}(k) - \mathbf{u}(l) + \xi(k, \alpha) - \xi(l, \beta).$$

Here $\mathbf{R}_o^{k\alpha}$ and $\mathbf{R}_o^{l\beta}$ are the position vectors of atoms (k, α) and (l, β) in the ground state, $\mathbf{u}(k)$ and $\mathbf{u}(l)$ are the displacements of the centers of the k -th and the l -th unit cells, and $\xi(k, \alpha)$ and $\xi(l, \beta)$ are the displacements of atoms (k, α) and (l, β) relative to their unit cell centers, that is, lattice points.

4.2. Momentum flux density. The temperature in an N -body dynamics systems is generally defined as [Chen and Lee 2006]

$$T^\alpha = \left\langle \frac{\Delta V}{3k_B} \sum_{k=1}^n m^\alpha (\tilde{\mathbf{V}}^{k\alpha})^2 \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\alpha} - \mathbf{y}^\alpha) \right\rangle.$$

We see that the kinetic parts of momentum flux in Equations (3–1) and (3–3), caused by the thermal motion of atoms, are related to temperature. They depend only on the magnitude of the fluctuations of atoms. This implies

$$\bar{\mathbf{i}}_{\text{kin}}^\alpha + \bar{\tau}_{\text{kin}}^\alpha = -\gamma T^\alpha \mathbf{I} \quad \text{or} \quad \bar{\mathbf{i}}_{\text{kin}}^\alpha = -\gamma_1 T^\alpha \mathbf{I}, \quad \bar{\tau}_{\text{kin}}^\alpha = -\gamma_2 T^\alpha \mathbf{I},$$

with

$$\gamma_1 + \gamma_2 = \gamma, \quad \gamma = \frac{k_B}{\Delta V}.$$

Using the δ -function identity (see Appendix),

$$\begin{aligned} & \int_0^1 \delta(\mathbf{R}^k \lambda + \mathbf{R}^l (1 - \lambda) - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} \lambda + \Delta \mathbf{r}^{l\eta} (1 - \lambda) - \mathbf{y}^\alpha) d\lambda \\ &= \sum_{m=1}^{\infty} \frac{1}{m!} ((\mathbf{R}^k - \mathbf{R}^l) \cdot \nabla_{\mathbf{x}} + (\Delta \mathbf{r}^{k\xi} - \Delta \mathbf{r}^{l\eta}) \cdot \nabla_{\mathbf{y}^\alpha})^{m-1} \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha), \end{aligned}$$

we see that the potential momentum fluxes, Equations (3–2) and (3–4), are functions of a series of high order gradients, with zeroth order terms

$$\begin{aligned} (\bar{\mathbf{t}}_{\text{pot}}^\alpha)^0 &= - \left\langle \frac{1}{2} \sum_{k,l=1}^n \sum_{\xi,\eta=1}^v (\mathbf{R}^k - \mathbf{R}^l) \otimes \mathbf{f}_1^{l\eta k\xi} \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha) \right\rangle, \\ (\bar{\boldsymbol{\tau}}_{\text{pot}}^\alpha)^0 &= - \left\langle \frac{1}{2} \sum_{k,l=1}^n \sum_{\xi,\eta=1}^v (\Delta \mathbf{r}^{k\xi} - \Delta \mathbf{r}^{l\eta}) \otimes \mathbf{f}_1^{l\beta k\xi} \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha) \right\rangle \\ &\quad - \left\langle \frac{1}{2} \sum_{k=1}^n \sum_{\xi,\eta=1}^v (\Delta \mathbf{r}^{k\xi} - \Delta \mathbf{r}^{k\eta}) \otimes \mathbf{f}_2^{k\xi \eta} \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha) \right\rangle. \end{aligned}$$

Note that the sum of zeroth momentum flux, $(\bar{\mathbf{t}}_{\text{pot}}^\alpha)^0 + (\bar{\boldsymbol{\tau}}_{\text{pot}}^\alpha)^0$, is the atomic virial stress. Using the expressions for interatomic forces, $(\bar{\mathbf{t}}_{\text{pot}}^\alpha)^0$ and $(\bar{\boldsymbol{\tau}}_{\text{pot}}^\alpha)^0$ can be expressed as

$$(\bar{\mathbf{t}}_{\text{pot}}^\alpha(\mathbf{x}, t))^0 = \frac{1}{2(\Delta V)^2} \int_{V(\mathbf{x}')} \sum_{\beta=1}^v G(d^{\alpha\beta})(\mathbf{x} - \mathbf{x}') \otimes \mathbf{d}^{\alpha\beta} dV(\mathbf{x}'), \quad (4-1)$$

$$\begin{aligned} (\bar{\boldsymbol{\tau}}_{\text{pot}}^\alpha(\mathbf{x}, t))^0 &= \frac{1}{2(\Delta V)^2} \int_{V(\mathbf{x}')} \sum_{\beta=1}^v G(d^{\alpha\beta}) \mathbf{y}^{\alpha\beta'} \otimes \mathbf{d}^{\alpha\beta} dV(\mathbf{x}') \\ &\quad + \frac{1}{\Delta V} \sum_{\beta=1}^v G(y^{\alpha\beta}) \mathbf{y}^{\alpha\beta} \otimes \mathbf{y}^{\alpha\beta}, \quad (4-2) \end{aligned}$$

and the first order terms as

$$\begin{aligned} (\bar{\mathbf{t}}_{\text{pot}}^\alpha(\mathbf{x}, t))^1 &= \frac{1}{4} \nabla_{\mathbf{x}} \cdot \left(\frac{1}{(\Delta V)^2} \int_{V(\mathbf{x}')} (\mathbf{x} - \mathbf{x}') \sum_{\beta=1}^v G(d^{\alpha\beta})(\mathbf{x} - \mathbf{x}') \otimes \mathbf{d}^{\alpha\beta} dV(\mathbf{x}') \right) \\ &+ \frac{1}{4} \nabla_{\mathbf{y}^\alpha} \cdot \left(\frac{1}{(\Delta V)^2} \int_{V(\mathbf{x}')} \sum_{\beta=1}^v \mathbf{y}^{\alpha\beta'} G(d^{\alpha\beta})(\mathbf{x} - \mathbf{x}') \otimes \mathbf{d}^{\alpha\beta} dV(\mathbf{x}') \right), \quad (4-3) \end{aligned}$$

$$\begin{aligned} (\bar{\mathbf{t}}_{\text{pot}}^\alpha(\mathbf{x}, t))^1 &= \frac{1}{4} \nabla_{\mathbf{x}} \cdot \left(\frac{1}{(\Delta V)^2} \int_{V(\mathbf{x}')} (\mathbf{x} - \mathbf{x}') \sum_{\beta=1}^v G(d^{\alpha\beta}) \mathbf{y}^{\alpha\beta'} \otimes \mathbf{d}^{\alpha\beta} dV(\mathbf{x}') \right) \\ &+ \frac{1}{4} \nabla_{\mathbf{y}^\alpha} \cdot \left(\frac{1}{(\Delta V)^2} \int_{V(\mathbf{x}')} \sum_{\beta=1}^v \mathbf{y}^{\alpha\beta'} G(d^{\alpha\beta}) \mathbf{y}^{\alpha\beta'} \otimes \mathbf{d}^{\alpha\beta} dV(\mathbf{x}') \right) \\ &+ \frac{1}{4} \nabla_{\mathbf{y}^\alpha} \cdot \left(\frac{1}{\Delta V} \sum_{\beta=1}^v \mathbf{y}^{\alpha\beta} G(\mathbf{y}^{\alpha\beta}) \mathbf{y}^{\alpha\beta} \otimes \mathbf{y}^{\alpha\beta} \right), \quad (4-4) \end{aligned}$$

where

$$\begin{aligned} \mathbf{d}^{\alpha\beta}(\mathbf{x}, \mathbf{x}') &\equiv \mathbf{x}_o + \mathbf{u}(\mathbf{x}) + \mathbf{y}_o^\alpha + \xi(\mathbf{x}, \alpha) - (\mathbf{x}'_o + \mathbf{u}(\mathbf{x}') + \mathbf{y}_o^\beta + \xi(\mathbf{x}', \beta)), \\ \mathbf{y}^{\alpha\beta} &\equiv \mathbf{y}^\alpha - \mathbf{y}^\beta = \mathbf{y}_o^\alpha + \xi^\alpha(\mathbf{x}) - (\mathbf{y}_o^\beta + \xi^\beta(\mathbf{x})), \\ \mathbf{y}^{\alpha\beta'} &\equiv \mathbf{y}^\alpha - \mathbf{y}'^\beta = \mathbf{y}_o^\alpha + \xi^\alpha(\mathbf{x}) - (\mathbf{y}_o^\beta + \xi^\beta(\mathbf{x}')), \\ \mathbf{d}^{\alpha\beta} &\equiv |\mathbf{d}^{\alpha\beta}|, \\ \mathbf{y}^{\alpha\beta} &\equiv |\mathbf{y}^{\alpha\beta}|. \end{aligned}$$

Equations (4-1)–(4-4) are the zeroth and the first order *nonlinear nonlocal constitutive relations for the potential momentum flux density*. The independent variables are the lattice displacement $\mathbf{u}(\mathbf{x}, t)$ and the relative atomic displacements $\xi(\mathbf{x}, \alpha, t) \triangleq \xi^\alpha(\mathbf{x}, t)$.

4.3. Linear local momentum flux density. To derive the linear constitutive relations for the potential momentum flux density one may make the assumption of infinitesimal deformation, namely, $\mathbf{d}^{\alpha\beta} - \mathbf{d}_o^{\alpha\beta} \rightarrow 0$. Therefore, the internal atomic force density can be written as

$$\mathbf{f}_{\text{int}}^\alpha(\mathbf{x}) \approx \frac{1}{(\Delta V)^2} \int_{V(\mathbf{x}')} \sum_{\beta=1}^v \left(\mathbf{c}_o^{\alpha\beta}(\mathbf{x}_0, \mathbf{x}'_0) + c_1^{\alpha\beta}(\mathbf{x}_0, \mathbf{x}'_0) (\mathbf{d}^{\alpha\beta} - \mathbf{d}_o^{\alpha\beta}) \right) dV(\mathbf{x}'),$$

where $\mathbf{d}_o^{\alpha\beta} = \mathbf{d}^{\alpha\beta}(\mathbf{x}_0, \mathbf{x}'_0)$ is the separate vector between two ground-state atoms, and $\mathbf{c}_o^{\alpha\beta}(\mathbf{x}_0, \mathbf{x}'_0) = c_1^{\alpha\beta} \mathbf{d}_o^{\alpha\beta}$ and $c_1^{\alpha\beta}$ are the interatomic force constants which can be computed from quantum mechanics and are functions of the type of atoms in

question as well as their separation. For the sake of simplicity, one may write

$$c_{0,1}^{\alpha\beta'} = c_{0,1}^{\alpha\beta}(\mathbf{x}_0, \mathbf{x}'_0), \quad c_{0,1}^{\alpha\beta} = c_{0,1}^{\alpha\beta}(\mathbf{x}_0, \mathbf{x}_0).$$

Using linearized atomic force, Equations (4-1)–(4-4) become

$$\begin{aligned} (\bar{\mathbf{t}}_{\text{pot}}^\alpha(\mathbf{x}, t))^0 &= \frac{1}{2(\Delta V)^2} \int_{V(\mathbf{x}')} \sum_{\beta=1}^{\nu} (\mathbf{x} - \mathbf{x}') \otimes (\mathbf{c}_o^{\alpha\beta'} + c_1^{\alpha\beta'} (\mathbf{d}^{\alpha\beta} - \mathbf{d}_o^{\alpha\beta})) dV(\mathbf{x}'), \\ (\bar{\mathbf{t}}_{\text{pot}}^\alpha(\mathbf{x}, t))^1 &= \frac{1}{4(\Delta V)^2} \nabla_x \cdot \int_{V(\mathbf{x}')} \sum_{\beta=1}^{\nu} (\mathbf{x} - \mathbf{x}') (\mathbf{x} - \mathbf{x}') \\ &\quad \otimes (\mathbf{c}_o^{\alpha\beta'} + c_1^{\alpha\beta'} (\mathbf{d}^{\alpha\beta} - \mathbf{d}_o^{\alpha\beta})) dV(\mathbf{x}') \\ &\quad + \frac{1}{4(\Delta V)^2} \nabla_{y^\alpha} \cdot \int_{V(\mathbf{x}')} \sum_{\beta=1}^{\nu} \mathbf{y}^{\alpha\beta'} (\mathbf{x} - \mathbf{x}') \\ &\quad \otimes (\mathbf{c}_o^{\alpha\beta'} + c_1^{\alpha\beta'} (\mathbf{d}^{\alpha\beta} - \mathbf{d}_o^{\alpha\beta})) dV(\mathbf{x}'), \\ (\bar{\tau}_{\text{pot}}^\alpha(\mathbf{x}, t))^0 &= \frac{1}{2(\Delta V)^2} \int_{V(\mathbf{x}')} \sum_{\beta=1}^{\nu} \mathbf{y}^{\alpha\beta'} \otimes (\mathbf{c}_o^{\alpha\beta'} + c_1^{\alpha\beta'} (\mathbf{d}^{\alpha\beta} - \mathbf{d}_o^{\alpha\beta})) dV(\mathbf{x}') \\ &\quad + \frac{1}{2\Delta V} \sum_{\beta=1}^{\nu} \mathbf{y}^{\alpha\beta} \otimes (\mathbf{c}_o^{\alpha\beta} + c_1^{\alpha\beta} (\mathbf{y}^{\alpha\beta} - \mathbf{y}_o^{\alpha\beta})), \\ (\bar{\tau}_{\text{pot}}^\alpha(\mathbf{x}, t))^1 &= \frac{1}{4(\Delta V)^2} \nabla_x \cdot \int_{V(\mathbf{x}')} (\mathbf{x} - \mathbf{x}') \sum_{\beta=1}^{\nu} \mathbf{y}^{\alpha\beta'} \otimes (\mathbf{c}_o^{\alpha\beta'} + c_1^{\alpha\beta'} (\mathbf{d}^{\alpha\beta} - \mathbf{d}_o^{\alpha\beta})) dV(\mathbf{x}') \\ &\quad + \frac{1}{4(\Delta V)^2} \nabla_{y^\alpha} \cdot \int_{V(\mathbf{x}')} \sum_{\beta=1}^{\nu} \mathbf{y}^{\alpha\beta'} \mathbf{y}^{\alpha\beta'} \otimes (\mathbf{c}_o^{\alpha\beta'} + c_1^{\alpha\beta'} (\mathbf{d}^{\alpha\beta} - \mathbf{d}_o^{\alpha\beta})) dV(\mathbf{x}') \\ &\quad + \frac{1}{4(\Delta V)} \nabla_{y^\alpha} \cdot \sum_{\beta=1}^{\nu} \mathbf{y}^{\alpha\beta} \mathbf{y}^{\alpha\beta} \otimes (\mathbf{c}_o^{\alpha\beta} + c_1^{\alpha\beta} (\mathbf{y}^{\alpha\beta} - \mathbf{y}_o^{\alpha\beta})). \end{aligned}$$

Note that material properties should make the ground state stresses vanish: $\bar{\mathbf{t}}_{\text{pot}}^\alpha(0) = \mathbf{0}$, $\bar{\tau}_{\text{pot}}^\alpha(0) = 0$. Hence, the expressions for potential momentum flux in the ground state

$$\begin{aligned} \bar{\mathbf{t}}_{\text{pot}}^\alpha(0) &= \frac{1}{2(\Delta V)^2} \int_{V(\mathbf{x}')} \sum_{\beta=1}^{\nu} (\mathbf{x}_o - \mathbf{x}'_o) \otimes \mathbf{c}_o^{\alpha\beta'} dV(\mathbf{x}'), \\ \bar{\tau}_{\text{pot}}^\alpha(0) &= \frac{1}{2(\Delta V)^2} \int_{V(\mathbf{x}')} \sum_{\beta=1}^{\nu} \mathbf{y}_o^{\alpha\beta} \otimes \mathbf{c}_o^{\alpha\beta'} dV(\mathbf{x}') + \frac{1}{\Delta V} \sum_{\beta=1}^{\nu} \mathbf{y}_o^{\alpha\beta} \otimes \mathbf{c}_o^{\alpha\beta}, \end{aligned}$$

can be used for validation once the material parameters $\mathbf{c}_0^{\alpha\beta'}$, $\mathbf{c}_0^{\alpha\beta}$ and the ground state structural parameters \mathbf{x}_o and $\mathbf{y}_o^{\alpha\beta}$ are obtained from quantum mechanical calculations.

If one further neglects nonlocal effects considering only the interactions between unit cells in a close neighborhood, one then has

$$\begin{aligned}\mathbf{u}(\mathbf{x}) - \mathbf{u}(\mathbf{x}') &\approx \mathbf{u}_{,x} \cdot (\mathbf{x}_o - \mathbf{x}'), \\ \xi(\mathbf{x}, \beta) - \xi(\mathbf{x}', \beta) &\approx \xi_{,x}^\beta \cdot (\mathbf{x}_o - \mathbf{x}'), \\ \xi(\mathbf{x}, \alpha) - \xi(\mathbf{x}, \beta) &\triangleq \gamma^{\alpha\beta} \cdot (\mathbf{y}_o^\alpha - \mathbf{y}_o^\beta),\end{aligned}$$

and hence

$$(\mathbf{x} - \mathbf{x}') - (\mathbf{x}_o - \mathbf{x}'_o) = \mathbf{u}(\mathbf{x}) - \mathbf{u}(\mathbf{x}') \approx \mathbf{u}_{,x} \cdot (\mathbf{x}_o - \mathbf{x}'_o), \quad (4-5)$$

$$(\mathbf{y}^\alpha - \mathbf{y}^\beta) - (\mathbf{y}_o^\alpha - \mathbf{y}_o^\beta) = \xi(\mathbf{x}, \alpha) - \xi(\mathbf{x}, \beta) \triangleq \gamma^{\alpha\beta} \cdot (\mathbf{y}_o^\alpha - \mathbf{y}_o^\beta), \quad (4-6)$$

$$\begin{aligned}(\mathbf{y}^\alpha - \mathbf{y}'^\beta) - (\mathbf{y}_o^\alpha - \mathbf{y}'_o^\beta) &= \xi(\mathbf{x}, \alpha) - \xi(\mathbf{x}', \beta) \\ &= \xi(\mathbf{x}, \alpha) - \xi(\mathbf{x}, \beta) + \xi(\mathbf{x}, \beta) - \xi(\mathbf{x}', \beta) \\ &\approx \gamma^{\alpha\beta} \cdot (\mathbf{y}_o^\alpha - \mathbf{y}_o^\beta) + \xi_{,x}^\beta \cdot (\mathbf{x}_o - \mathbf{x}'_o),\end{aligned} \quad (4-7)$$

$$\mathbf{d}^{\alpha\beta} - \mathbf{d}_0^{\alpha\beta} \approx (\mathbf{u}_{,x} + \xi_{,x}^\beta) \cdot (\mathbf{x}_o - \mathbf{x}'_o) + \gamma^{\alpha\beta} \cdot (\mathbf{y}_o^\alpha - \mathbf{y}_o^\beta). \quad (4-8)$$

The zeroth order linear local potential momentum flux density can be then expressed as

$$\bar{\mathbf{t}}^\alpha(\mathbf{x}, t) = -\gamma_1 T^\alpha \mathbf{I} + \sum_{\beta=1}^v (\mathbf{A}^1 : \mathbf{u}_{,x} + \mathbf{A}^2 : \gamma^{\alpha\beta} + \mathbf{A}^3 : \xi_{,x}^\beta), \quad (4-9)$$

$$\bar{\mathbf{t}}^\alpha(\mathbf{x}, t) = -\gamma_2 T^\alpha \mathbf{I} + \sum_{\beta=1}^v (\mathbf{B}^1 : \mathbf{u}_{,x} + \mathbf{B}^2 : \gamma^{\alpha\beta} + \mathbf{B}^3 : \xi_{,x}^\beta). \quad (4-10)$$

Here $(\mathbf{A} : \mathbf{B})_{ijk\dots lmn} = A_{ijk\dots pq} B_{pq\dots lmn}$.

Note that $\mathbf{d}_0^{\alpha\beta}$, $\mathbf{x}_o - \mathbf{x}'_o$, and $\mathbf{y}_o^{\alpha\beta} = \mathbf{y}_o^\alpha - \mathbf{y}_o^\beta$ are material constants, while $\mathbf{d}^{\alpha\beta}$, $\mathbf{x} - \mathbf{x}'$ and $\mathbf{y}^\alpha - \mathbf{y}^\beta$ are up to first order in $\mathbf{u}_{,x}$, $\xi_{,x}^\beta$, and $\gamma^{\alpha\beta}$. Using Equations (4-5)–(4-8) one can find that the first order terms of momentum flux density are the strain gradient terms. Therefore, Equations (4-9) and (4-10) represent the linear local form of zeroth order homogeneous and inhomogeneous momentum flux density, and the sum of the two is the field representation of atomic virial

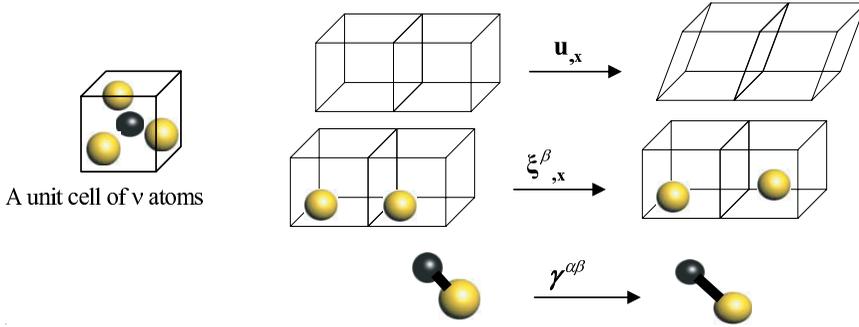


Figure 5. Illustration of strain measures in the formulated field theory.

stress. One can also write them in tensor notation as:

$$\bar{t}_{mn}^{\alpha}(\mathbf{x}, t) = -\gamma_1^{\delta mn} T^{\alpha} + \sum_{\beta=1}^{\nu} (A_{mnpq}^1 \varepsilon_{pq}^1 + A_{mnpq}^2 \varepsilon_{pq}^2 + A_{mnpq}^3 \varepsilon_{pq}^3),$$

$$\bar{\tau}_{mn}^{\alpha}(\mathbf{x}, t) = -\gamma_2^{\delta mn} T^{\alpha} + \sum_{\beta=1}^{\nu} (B_{mnpq}^1 \varepsilon_{pq}^1 + B_{mnpq}^2 \varepsilon_{pq}^2 + B_{mnpq}^3 \varepsilon_{pq}^3),$$

where

$$\varepsilon_{pq}^1 = u_{p,q}, \quad \varepsilon_{pq}^2 = \gamma_{pq}^{\alpha\beta}, \quad \varepsilon_{pq}^3 = \xi_{p,q}^{\beta}, \quad (4-11)$$

and

$$A_{mnpq}^{i=1,2,3}, \quad B_{mnpq}^{i=1,2,3}$$

are material constants which can be expressed in terms of ground state structural parameters $\mathbf{x}_o - \mathbf{x}'_o$, $\mathbf{y}_o^{\alpha} - \mathbf{y}_o^{\beta}$ and a material parameter $c_1^{\alpha\beta}$.

4.4. Strain measures. The field representation of momentum flux involves temperature, lattice deformation and relative atomic deformation. The linear local forms of momentum flux are expressed in terms of temperature and lattice strain $\mathbf{u}_{,x}(\mathbf{x})$, relative atomic strain $\xi_{,x}^{\beta}(\mathbf{x})$, and atomic-bond strain $\gamma^{\alpha\beta}(\mathbf{x})$. They are the lattice deformation gradient, relative atomic deformation gradient and relative atomic-bond stretch, and can be illustrated through Figure 5.

5. Numerical examples

For the purpose of numerical validation, a periodic solid under simple tension is modeled and simulated. Stress and strain relations are computed based on the formulas derived in this paper and by atomic-level molecular dynamics simulation (MD) as well. The general-purpose parallel MD simulation code DL-POLY is employed [Smith and Forester 2001] to perform the simulation. The modeling of simple tension is achieved through NVT ensemble.

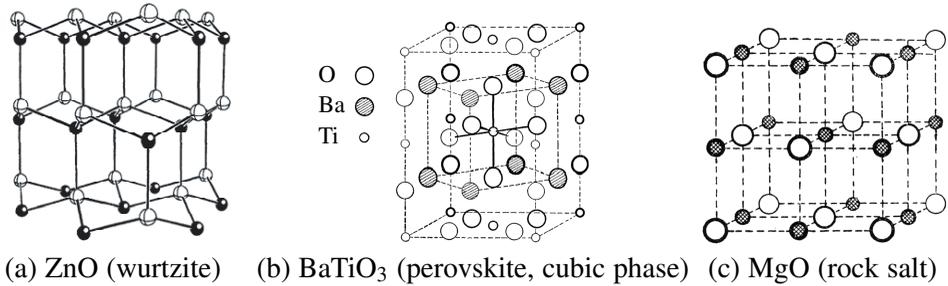


Figure 6. Crystal structure of zinc oxide, barium titanate, and magnesium oxide.

Three single crystalline materials are considered in this paper. Among them, piezoelectric and semiconductor material Zinc Oxide, ZnO, is wurtzite structured with lattice constants $a = 3.249 \text{ \AA}$ and $c = 5.206 \text{ \AA}$, ferroelectric material Barium Titanate, BaTiO₃ is in its cubic phase with the lattice constant $a = 3.943 \text{ \AA}$, and MgO, the standard test-bed material for the evaluation of theoretical methods to calculate some mechanical properties, has a rock salt structure with the lattice constant $a = 4.2 \text{ \AA}$. The Coulomb and Buckingham interatomic potentials are employed for the MD simulation, and the material parameters are taken from [Catlow 1986; Grimes 1994; McCoy et al. 1997a; 1997b; Grimes et al. 1995; Chen et al. 1997].

Under uniform simple tension loading, there are no strain gradients, and hence only the zeroth momentum flux exists. Thus, the formula for the total stress reduces to the zeroth order momentum flux, $(\vec{\tau}_{\text{pot}}^\alpha)^0 + (\bar{\tau}_{\text{pot}}^\alpha)^0$, which is identical to the atomic virial stress.

The numerical results of the stress-strain relations before the onset of structure stability (phase transition) by the formulation and DL-POLY are plotted in Figure 7. A good agreement between the results from the formulation and from the DL-POLY simulation is found, while the computational time ratio between these two methods is about 1 to 10^4 . Although the analytical stress-strain relation is nonlinear and nonlocal, surprisingly the numerical results indicate that the stress-strain relation is quite linear until structural transformation.

6. Summary and discussion

The field representation of momentum flux density is formulated in this paper within the framework of atomic N -body dynamics. Three strain measures and the momentum flux density–strain relations are obtained. Major considerations and conclusions regarding the formulation may be summarized as follows:

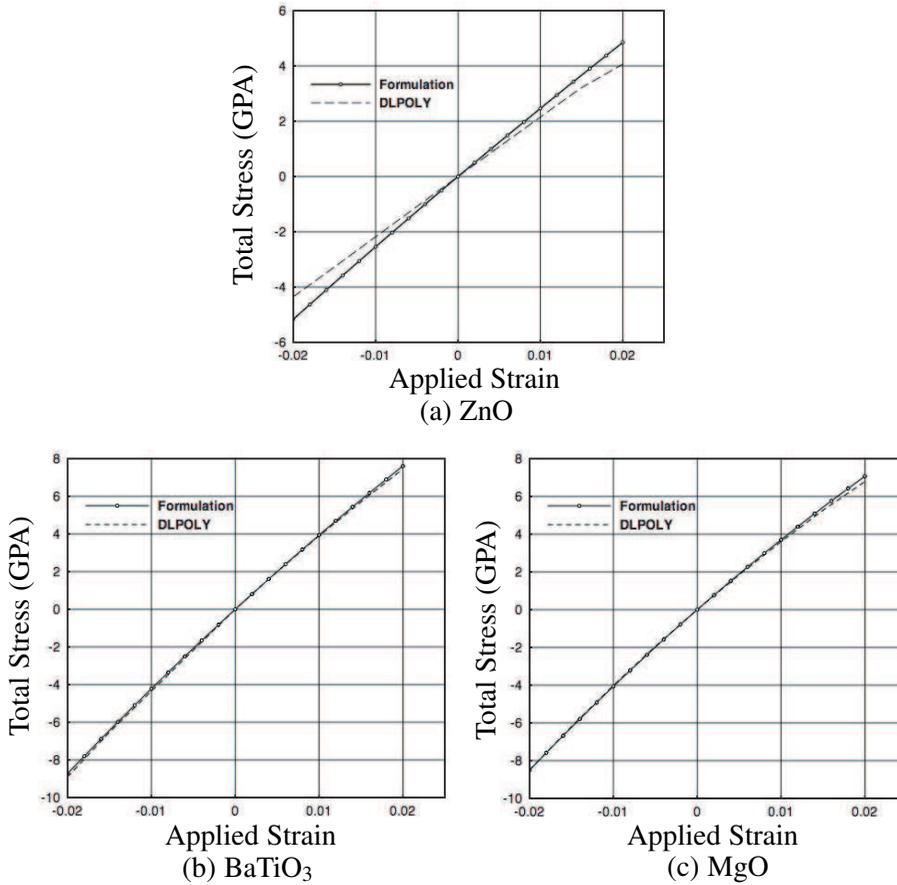


Figure 7. Stress-strain relation of zinc oxide (a), barium titanate (b), and magnesium oxide (c) by the formulation and by molecular dynamics simulation code DL-POLY.

- (1) The momentum flux formulated in this paper exactly represents the momentum flux in an atomic N -body dynamics model. Both the atomic-level momentum flux and the atomic displacements can be fully represented in terms of field variables: temperature, lattice deformation and relative atomic deformation. All material constants involved can be obtained through the atomistic formulation.
- (2) This paper has shown that the stress in the conventional continuum description is not the momentum flux density in an atomic N -body dynamics model; it is only the homogeneous part of momentum flux density summing over at least the volume of a primitive unit cell. Decomposing the momentum flux into homogeneous and inhomogeneous parts, one can establish the connection

between the atomic momentum flux density and the continuum stress, and obtain the field representation of conservation equations on the atomic scale [Chen and Lee 2006].

- (3) The formulations have shown that the momentum flux density-strain relation, which may be referred to as atomic stress-strain relation, is nonlinear and nonlocal in displacements, and involves higher order gradients. In the case of homogeneous strain so that no strain gradients exist, the formula for total stress shall be identical to the virial theorem. Or, if the average stress of a whole specimen is concerned, then the total stress formula shall also be identical to the virial theorem.
- (4) The three strain measures are obtained for the linear local constitutive relation. One may prove that the nonlinear nonlocal relation can also be expressed in terms of the temperature and the three strain measures.
- (5) The numerical examples in this paper, although quite preliminary, show that the stress-strain relation under uniform loading is linear until structural instability.

Appendix

Define

$$\begin{aligned}\delta(\lambda; k, l, \xi, \eta, \alpha) &\equiv \delta(\mathbf{R}^k \lambda + \mathbf{R}^l (1 - \lambda) - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} \lambda + \Delta \mathbf{r}^{l\eta} (1 - \lambda) - \mathbf{y}^\alpha) \triangleq \delta(\lambda), \\ \Delta(k, \xi, \alpha) &\equiv \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha) \triangleq \Delta = \delta(1), \\ A &\equiv (\mathbf{R}^k - \mathbf{R}^l) \cdot \nabla_{\mathbf{x}}, \\ B &\equiv (\Delta \mathbf{r}^{k\xi} - \Delta \mathbf{r}^{l\eta}) \cdot \nabla_{\mathbf{y}^\alpha}.\end{aligned}$$

It is readily verified that

$$\begin{aligned}\frac{d\delta}{d\lambda} &= -(A + B)\delta, \\ d\delta &= -(A + B)\delta d\lambda, \\ \int_0^1 \lambda \frac{d\delta}{d\lambda} d\lambda &= \int_0^1 \lambda d\delta = \lambda \delta \Big|_0^1 - \int_0^1 \delta d\lambda = \delta(1) - \int_0^1 \delta d\lambda, \\ \int_0^1 \delta d\lambda &= \Delta + (A + B) \int_0^1 \lambda \delta d\lambda, \\ \int_0^1 \lambda^n d\delta &= \Delta - n \int_0^1 \lambda^{n-1} \delta d\lambda,\end{aligned}$$

which gives

$$\int_0^1 \lambda^{n-1} \delta d\lambda = \frac{\Delta}{n} + \frac{1}{n}(A+B) \int_0^1 \lambda^n \delta d\lambda.$$

One may then prove that

$$\begin{aligned} \int_0^1 \delta d\lambda &= \Delta + (A+B) \int_0^1 \lambda \delta d\lambda \\ &= \Delta + (A+B) \left(\frac{\Delta}{2} + \frac{1}{2}(A+B) \int_0^1 \lambda^2 \delta d\lambda \right) \\ &= \Delta + \frac{1}{2}(A+B)\Delta + \frac{1}{2}(A+B)^2 \int_0^1 \lambda^2 \delta d\lambda \\ &= \dots = \sum_{n=1}^{\infty} \frac{1}{n!} (A+B)^{n-1} \Delta, \end{aligned}$$

or, in other words,

$$\begin{aligned} \int_0^1 \delta(\mathbf{R}^k \lambda + \mathbf{R}^l (1-\lambda) - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} \lambda + \Delta \mathbf{r}^{l\eta} (1-\lambda) - \mathbf{y}^\alpha) d\lambda \\ = \sum_{m=1}^{\infty} \frac{1}{m!} ((\mathbf{R}^k - \mathbf{R}^l) \cdot \nabla_{\mathbf{x}} + (\Delta \mathbf{r}^{k\xi} - \Delta \mathbf{r}^{l\eta}) \cdot \nabla_{\mathbf{y}^\alpha})^{m-1} \delta(\mathbf{R}^k - \mathbf{x}) \delta(\Delta \mathbf{r}^{k\xi} - \mathbf{y}^\alpha), \\ \int_0^1 \delta(\mathbf{R}^k \lambda + \mathbf{R}^l (1-\lambda) - \mathbf{x}) d\lambda = \sum_{m=1}^{\infty} \frac{1}{m!} ((\mathbf{R}^k - \mathbf{R}^l) \cdot \nabla_{\mathbf{x}})^{m-1} \delta(\mathbf{R}^k - \mathbf{x}). \end{aligned}$$

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Received 4 Dec 2005.

YOUPING CHEN: ypchen2@gwu.edu

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

JAMES LEE: jdlee@gwu.edu

The George Washington University, Academic Center T733, 801 22nd street, NW, Washington, DC 20052, United States

LIMING XIONG: xlm@gwu.edu

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

