Atomistic viewpoint of the applicability of microcontinuum theories

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Abstract

Microcontinuum field theories, including Micromorphic theory, Microstructure theory, Micropolar theory, Cosserat theory, nonlocal theory and couple stress theory, are the extensions of the classical field theories for the applications in microscopic space and time scales. They have been expected to overlap atomic model at microscale and encompass classical continuum mechanics at macroscale. This work provides an atomic viewpoint to examine the physical foundations of those well-established microcontinuum theories, and to justify their applicability through lattice dynamics and molecular dynamics.
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1. Introduction

Continuum theories describe a system in terms of a few variables such as mass, temperature, voltage and stress, which are suited directly to measurements and senses. Their successes, expediency and practicality, have been demonstrated and tested throughout the history of science in explaining and predicting diverse physical phenomena.

To explain the fundamental departure of microcontinuum theories from the classical continuum theories, the former is a continuum model embedded with microstructures to describe the microscopic motion, or a nonlocal model to describe the long-range material interaction. This extends the application of the continuum model to microscopic space and short-time scales. Micromorphic theory (Eringen and Suhubi, 1964; Eringen, 1999) treats a material body as a continuous collection of a large number of deformable particles, with each particle possessing finite size and inner structure. Using assumptions such as infinitesimal deformation and slow motion, Micromorphic theory can be reduced to Mindlin's Microstructure theory (1964). When the microstructure of the material is considered rigid, it becomes the Micropolar

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theory (Eringen and Suhubi, 1964). Assuming a constant microinertia, 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 becomes couple stress theory (Mindlin and Tiersten, 1962; Toupin, 1962). When the particle reduces to the mass point, all the theories reduce to the classical or ordinary continuum mechanics.

The physical world is composed of atoms moving under the influence of their mutual interaction forces. These interactions at microscopic scale are the physical origin of many macroscopic phenomena. Atomistic investigation helps to identify macroscopic quantities and their correlations, and enhance our understanding of various physical theories. This paper aims to analyze the applicability of those well-established microcontinuum theories from the atomistic viewpoint of lattice dynamics and molecular dynamics.

2. Applicability analyses from the viewpoint of dynamics of atoms in crystal

2.1. Dynamics of atoms in crystal

Some material features, such as chemical properties, material hardness, material symmetry, can be explained by static atomic structure. However, a large number of technically important properties can only be understood on the basis of lattice dynamics. These include temperature effect, energy dissipation, sound propagation, phase transition, thermal conductivity, piezoelectricity, dielectric and optical properties, and thermo-mechanical-electromagnetic coupling properties.

The atomic motions, revealed by those features, are not random. In fact they are determined by the forces that atoms exert on each other, and most readily described not in terms of the vibrations of individual atoms, but in terms of traveling waves, as illustrated in Fig. 1. Those waves are the normal modes of vibration of the system. The quantum of energy in an elastic wave is called a Phonon; a quantum state of a crystal lattice near its ground state can be specified by the phonons present; at very low temperature a solid can be regarded as a volume containing noninteracting phonons. The frequency–wave vector relationship of phonons is called phonon dispersion relation, which is the fundamental ingredient in the theory of lattice dynamics and can be determined through experimental measurements, such as neutron scattering, infrared spectroscope and Raman scattering, or first principle calculations or phenomenological modeling. Through phonon dispersion relations, the dynamic characteristics of an atomic system can be represented, the validity of a calculation or a phenomenological modeling can be examined, interatomic force constants can be computed, and various material parameters can be determined.

2.2. Optical phonons

Optical phonon branches exist in all crystals with more than one atom per primitive unit cell. In such crystals, the elastic distortions produce wave propagation of two types: In the acoustic type (as LA and TA), all the atoms in the unit cell move in essentially the same phase, resulting in the deformation of lattice, usually referred to as homogeneous deformation. In the optical type (as LO and TO), the atoms move within the unit cell, leave the unit cell unchanged, contribute to the discrete feature of an atomic system, and give rise to the internal deformations. In an optical vibration of noncentral ionic crystal, the relative displacement between the positive and negative ions gives rise to the piezoelectricity. Optics is a
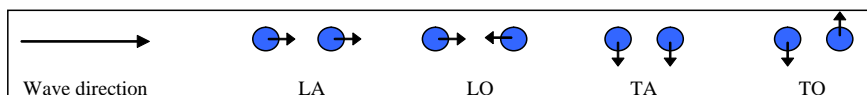

Fig. 1. Typical motions for two atoms in a unit cell, where "L" stands for longitudinal, "T" transverse, "A" acoustic, "O" optical.

phenomenon that necessitates the presence of an electromagnetic field. In ABO_3 ferroelectrics the anomalously large Born effective charges produce a giant LO–TO splitting in phonon dispersion relations. This feature is associated with the existence of an anomalously large destabilizing dipole–dipole interaction, sufficient to compensate the stabilizing short-range force and induce the ferroelectric instability. Optical phonon, therefore, appears as the key concept to relate the electronic and structural properties through Born effective charge (Ghosez et al., 1995; Ghosez, 1997). The elastic theory of continuum is the long-wave limit of acoustic vibrations of lattice, while optical vibrations explain many macroscopic phenomena involving thermal, mechanical, electromagnetic and optical coupling effects.

2.3. Dynamic feature of various types of crystals

The dynamic characteristics of crystals depend on crystal structures, as shown in Fig. 2, and the binding between the atoms. In metals the atomic cores are surrounded by a more-or-less uniform density of free electrons. This gives metals their electrical conductivity and a nonlocal character of the interatomic potential. Its dynamic feature is represented by the dispersive acoustic vibrations. In ionic crystals, strong Coulomb forces and short-range repulsive forces operate between the ions, and the ions are polarizable. The covalent bond is usually formed from two electrons, one from each atom participating in the bond. These electrons tend to be partially localized in the region between the two atoms and constitute the bond charge. The phonon dispersion relations of ionic and covalent crystals have both acoustic and optical branches. Their optical vibrations describe the internal motion of atoms within the primitive basis, as in Figs. 1 and 3. In molecular crystal there is usually a large difference between the frequencies of modes in which the molecules move as united units (the external modes) and the modes that involve the stretch and distortion of the molecules (the internal modes). The framework crystals are similar to molecular crystals in that they are composed of rigid groups. The units are very stiff but linked flexibly to each other at the corner atoms. The phonon dispersion relations, as in Fig. 4, of molecular and framework crystals include both acoustic and optical vibrations, and the optical vibrations further include internal modes and external modes.

2.4. Phonon dispersion relations by various microcontinuum theories

2.4.1. Micromorphic theory (Eringen and Suhubi, 1964; Eringen, 1999)
Micromorphic theory views a material as a continuous collection of deformable particles. Each particle is attached with a microstructure of finite size. The deformation of a micromorphic continuum yields both
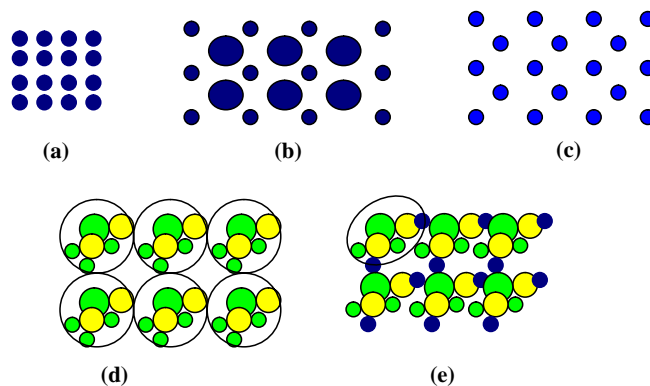

Fig. 2. Illustrations of crystal structures: (a) metallic crystal, (b) ionic crystal, (c) covalent crystal, (d) molecular crystal and (e) framework crystal.
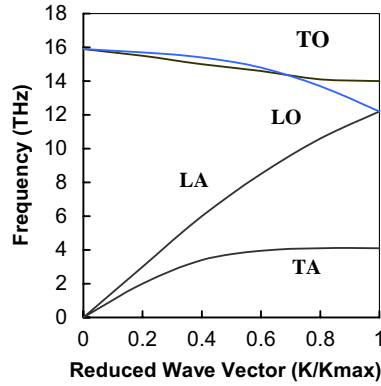
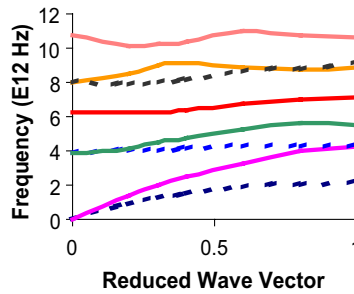Fig. 3. Phonon dispersion relations of silicon.

Fig. 4. Phonon dispersion relations of quartz (first 8 modes). Solid lines: symmetric modes, dot lines: anti-symmetric modes.

macrostrains (homogeneous part) and microscopic internal strains (inhomogeneous part) as shown in Fig. 5.

For isotropic elastic solids the stress–strain relations of Micromorphic theory are written as (Chen and Lee, 2003a)

$$t_{ij} = a_{ijkl}\gamma_{kl} + d_{ijkl}\eta_{kl} = a_1\delta_{ij}\gamma_{kk} + a_2\gamma_{ij} + a_3\gamma_{ji} + d_1\delta_{ij}\eta_{kk} + d_2(\eta_{ij} + \eta_{ji}), \tag{1}$$

$$m_{ijk} = c_{ijklmn}\lambda_{lmn}$$
$$= c_1\delta_{ij}\lambda_{kmn} + c_2\delta_{ij}\lambda_{mkm} + c_3\delta_{ij}\lambda_{mmk} + c_1\delta_{ik}\lambda_{jmm} + c_5\delta_{ik}\lambda_{mjm} + c_2\delta_{ik}\lambda_{mmj} + c_7\delta_{jk}\lambda_{imm} + c_8\lambda_{ijk}$$
$$+ c_9\lambda_{ikj} + c_1\delta_{jk}\lambda_{mim} + c_2\lambda_{kij} + c_3\lambda_{jik} + c_1\delta_{jk}\lambda_{mmi} + c_5\lambda_{kji} + c_2\lambda_{jki}, \tag{2}$$
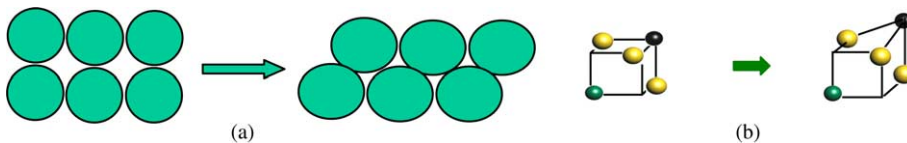

Fig. 5. Displacements in Micromorphic theory: (a) the displacements of the center of particles and (b) the microscopic internal displacement within the microstructure of a particle.

$$s_{ij} = b_{ijkl}\eta_{kl} + d_{klij}\gamma_{kl} = b_1\delta_{ij}\eta_{kk} + b_2(\eta_{ij} + \eta_{ji}) + d_1\delta_{ij}\gamma_{kk} + d_2(\gamma_{ij} + \gamma_{ji}), \tag{3}$$

which involves 14 elastic constants. The strains are related to the macrodisplacements u_i and internal deformation ϕ_{ij} as

$$\gamma_{ij} = u_{j,i} - \phi_{ji}, \tag{4}$$

$$\eta_{ij} = \eta_{ji} = \frac{1}{2}(\phi_{ij} + \phi_{ji}), \tag{5}$$

$$\lambda_{ijk} = \phi_{jk,i}. \tag{6}$$

Assuming harmonic waves propagating along the x-direction as,

$$u_i = iU_i e^{i(kx - \omega t)}, \tag{7}$$

$$\phi_{ij} = \Phi_{ij} e^{i(kx - \omega t)}, \tag{8}$$

the phonon dispersion relations can be obtained and grouped as follows:

(1) longitudinal external rotational optical wave (LRO)

$$(Ak^2 + B - \rho j\omega^2)\Phi_{[23]} = 0, \tag{9}$$

(2) transverse internal shear optical waves (TSO)

$$(\overline{A}k^2 + \overline{B} - \rho j\omega^2)(\Phi_{(23)}; \Phi_{22} - \Phi_{33}) = 0, \tag{10}$$

(3) longitudinal acoustic, longitudinal internal optical and dilatational optical waves (LA, LO, LDO)

$$\begin{vmatrix} A_{11}k^2 - \rho\omega^2 & A_{12}k & A_{13}k \\ A_{12}k & A_{22}k^2 + B_{22} - \frac{3}{2}\rho j\omega^2 & A_{23}k^2 \\ A_{13}k & A_{23}k^2 & A_{33}k^2 + B_{33} - 3\rho j\omega^2 \end{vmatrix} \begin{Vmatrix} U_1 \\ \Phi_{11}^d \\ \Phi \end{Vmatrix} = 0, \tag{11}$$

(4) transverse acoustic, transverse internal optical, and transverse external rotational optical waves (TA, TO, TRO)

$$\begin{vmatrix} \overline{A}_{11}k^2 - \rho\omega^2 & \overline{A}_{12}k & \overline{A}_{13}k \\ \overline{A}_{12}k & \overline{A}_{22}k^2 + \overline{B}_{22} - 2\rho j\omega^2 & \overline{A}_{23}k^2 \\ \overline{A}_{13}k & \overline{A}_{23}k^2 & \overline{A}_{33}k^2 + \overline{B}_{33} - 2\rho j\omega^2 \end{vmatrix} \begin{Vmatrix} U_2 & U_3 \\ \Phi_{(12)} & \Phi_{(13)} \\ \Phi_{[12]} & \Phi_{[13]} \end{Vmatrix} = 0, \tag{12}$$

where ρ is the mass density; j the microinertia; A, A_{ij}, $\overline{A}_{ij}$, B, $\overline{B}$, B_{ij}, $\overline{B}_{ij}$ are linearly related to the elastic constants; and

$$\Phi_{(ij)} \equiv \frac{1}{2}(\Phi_{ij} + \Phi_{ji}), \tag{13}$$

$$\Phi_{[ij]} \equiv \frac{1}{2}(\Phi_{ij} - \Phi_{ji}), \tag{14}$$

$$\Phi \equiv \frac{1}{3}(\Phi_{11} + \Phi_{22} + \Phi_{33}), \tag{15}$$

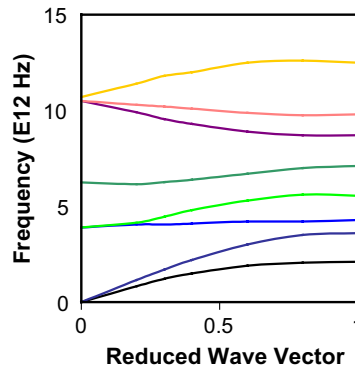$$\Phi_{11}^d \equiv \Phi_{11} - \Phi. \tag{16}$$

Fig. 6. Phonon dispersion relations calculated by micromorphic solid.

It is seen that the Micromorphic theory can provide up to 12 dispersion relations, including 3 acoustic, 9 optical (internal and external) modes. It can, therefore, describe the dynamic feature of (1) covalent and ionic crystals which only have acoustic and internal optical branches, and (2) molecular and framework crystals, in which both internal and external modes may exist (Fig. 6).

Mindlin's microstructure theory is a linear elastic version of Micromorphic theory. It is identical to Micromorphic theory in the linear elastic case.

2.4.2. Micropolar theory (Eringen and Suhubi, 1964)

When the material particle is considered as rigid, i.e., neglecting the internal motion within the inner structure of the particle, Micromorphic theory becomes Micropolar theory. Therefore, Micropolar theory yields only acoustic and external optical modes. They are the translational and rotational modes of rigid units. For molecular crystals or framework crystal, or chopped composite, granular material etc., when the external modes in which the molecules move as rigid units have much lower frequencies and thus dominate the dynamics of atoms, Micropolar theory can give a good description. It accounts for the dynamic effect of material with rather stiff microstructure.

Assuming a constant microinertia, Micropolar theory is identical to Cosserat theory (1909). Compared with Micropolar theory, Cosserat theory is limited to problems not involving significant change of the orientation of the microstructure, such as liquid crystal and ferroelectric materials.

2.4.3. Nonlocal theory (Eringen, 1966; Edelen, 1969)

Nonlocal theories state that the stresses at a point x are not only functions of the strains at x, but also functions of strains at all points in the body. A simplest nonlocal theory has the following form:

$$\sigma_{ij}(x) = C_{ijkl}\varepsilon_{kl}(x) + \int c_{ijkl}(x, x')\varepsilon_{kl}(x')\,\mathrm{d}x'. \qquad (17)$$

The strain gradients appear after the performance of the integrations when $\varepsilon_{kl}(\mathbf{x}')$ is written as a Taylor series around point x. This is why strain gradient theories are sometimes called nonlocal theories.

For isotropic material, the phonon dispersion relations based on a nonlocal theory have been obtained by Eringen (1992) as shown in Fig. 7. Remarkable similarity to atomic lattice dynamics solution with the Born–von Karman model, and to the experimental results for aluminum has been reported.

Nonlocal theory considers long-range interatomic interaction and yields results dependent on the size of a body. Similar to classical Continuum theory, the lattice particles are taken without structure and idealized as point masses. Hence, the effect of microstructure does not appear. It is not a theory for material with
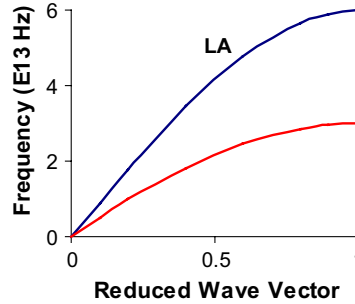
Fig. 7. Phonon dispersion relations by nonlocal theory.

microstructure, but for material involving long-range interaction. It can be applied to crystal that has only one atom per primitive unit cell at various length scales.

2.4.4. Couple stress theory (Mindlin and Tiersten, 1962; Toupin, 1962)

Couple stress theory (Mindlin and Tiersten, 1962; Toupin, 1962), by including high order stresses, yields results that depend on the specimen size. The constitutive relations for isotropic materials take the form

$$t_{ij} = \lambda e_{kk}\delta_{ij} + 2\mu e_{ij}, \tag{18}$$

$$m_{ijk} = \frac{1}{2}a_1(u_{i,mm}\delta_{jk} + 2u_{m,mk}\delta_{ij} + u_{j,mm}\delta_{ik}) + a_2(u_{m,mi}\delta_{jk} + u_{m,mj}\delta_{ik}) + 2a_3u_{k,mm}\delta_{ij} + 2a_4u_{k,ij}$$
$$+ a_5(u_{i,jk} + u_{j,ik}). \tag{19}$$

Assuming harmonic waves,

$$u_i(x,t) = U_i e^{i(kx-\omega t)}, \tag{20}$$

LA and TA dispersion relations result as

$$2(a_1 + a_2 + a_3 + a_4 + a_5)k^4 + (\lambda + 2\mu)k^2 = \rho\omega^2 + \rho j\omega^2 k^2, \tag{21}$$

$$2(a_3 + a_4)k^4 + \mu k^2 = \rho\omega^2 + \rho j\omega^2 k^2. \tag{22}$$

Both are dispersive, but acoustic waves only. The absence of optical branch is due to neglect of the atomic structure of crystal. From this viewpoint, the couple stress theories do not stem from the considerations of microstructure or microscopic internal motion.

3. Applicability analyses from the viewpoint of molecular dynamics

3.1. An atomic model of molecular dynamics

In a general case, consider a unit cell k in a crystal ($k = 1, 2, 3, \ldots, n$), each unit cell is composed of v atoms with the mass m^α ($\alpha = 1, 2, \ldots, v$), position $\mathbf{R}^{k\alpha}$ and the velocity $\mathbf{V}^{k\alpha}$. The mass m, coordinate $\mathbf{R}^k$ and velocity $\mathbf{V}^k$ at the center of the unit cell can be obtained as
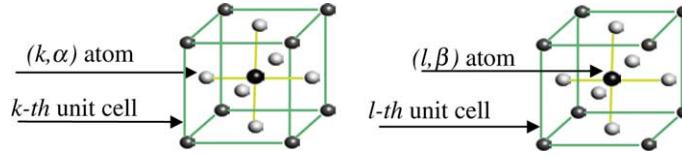
$$m = \sum_{\alpha=1}^{v} m^\alpha, \tag{23}$$

Fig. 8. Illustration of (k, α) and (l, β) atoms, atoms per unit cell $8 \times \frac{1}{8} + 6 \times \frac{1}{2} + 1 = 5$.

$$\boldsymbol{R}^k = \frac{1}{m} \sum_{\alpha=1}^{v} m^\alpha \boldsymbol{R}^{k\alpha}, \tag{24}$$

$$\boldsymbol{V}^k = \frac{1}{m} \sum_{\alpha=1}^{v} m^\alpha \boldsymbol{V}^{k\alpha}. \tag{25}$$

The relative positions and velocities between atoms and the center of the unit cell are

$$\Delta \boldsymbol{r}^{k\alpha} \equiv \boldsymbol{R}^{k\alpha} - \boldsymbol{R}^k, \quad \Delta \boldsymbol{v}^{k\alpha} \equiv \boldsymbol{V}^{k\alpha} - \boldsymbol{V}^k. \tag{26}$$

The interatomic forces can be derived from the potential functions. Three kinds of forces are assumed to act on an atom (Fig. 8):

1. $\boldsymbol{f}_1^{\substack{k\alpha \\ l\beta}}$: interatomic force between the (k, α) and (l, β) atoms, which correspond to the potential $u_1^{\substack{k\alpha \\ l\beta}}$, with

$$u_1^{\substack{k\alpha \\ l\beta}} = u_1^{\substack{l\beta \\ k\alpha}}, \tag{27}$$

$$\boldsymbol{f}_1^{\substack{k\alpha \\ l\beta}} = -\frac{\partial}{\partial \boldsymbol{R}^{k\alpha}} u_1^{\substack{k\alpha \\ l\beta}} = \frac{\partial}{\partial \boldsymbol{R}^{l\beta}} u_1^{\substack{k\alpha \\ l\beta}} = -\boldsymbol{f}_1^{\substack{l\beta \\ k\alpha}}. \tag{28}$$

2. $\boldsymbol{f}_2^{\substack{k\alpha \\ \beta}}$: interatomic force between the atoms α and β in the same unit cell k, which correspond to potential $u_2^{\substack{k\alpha \\ \beta}}$, with

$$u_2^{\substack{k\alpha \\ \beta}} = u_2^{\substack{k\beta \\ \alpha}}, \tag{29}$$

$$\boldsymbol{f}_2^{\substack{k\alpha \\ \beta}} = -\frac{\partial}{\partial \boldsymbol{R}^{k\alpha}} u_2^{\substack{k\alpha \\ \beta}} = \frac{\partial}{\partial \boldsymbol{R}^{k\beta}} u_2^{\substack{k\alpha \\ \beta}} = -\boldsymbol{f}_2^{\substack{k\beta \\ \alpha}}. \tag{30}$$

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

$$\boldsymbol{f} \equiv \sum_{\alpha=1}^{v} \boldsymbol{f}_3^{k\alpha} / \Delta V \tag{31}$$

and the body couple density

$$\boldsymbol{l} = \sum_{\alpha=1}^{v} \boldsymbol{f}_3^{k\alpha} \otimes \Delta \boldsymbol{r}^{k\alpha} / \Delta V. \tag{32}$$

3.2. Averaged field quantities from the atomic model

A continuum field quantity $\overline{A}(\boldsymbol{x}, t)$ in physical space is defined as the ensemble average of a dynamical function A in phase space with the following characteristic form (Balescu, 1975, 1997):

$$\overline{A} \equiv \langle A \rangle \equiv \int_p \int_r A(\mathbf{r}, \mathbf{p}, \mathbf{x}) f(\mathbf{r}, \mathbf{p}, t) \, d\mathbf{r} \, d\mathbf{p}, \tag{33}$$

where $\mathbf{r}$ is the position, $\mathbf{p}$ the momentum, f the normalized distribution function, i.e.,

$$\int \int f(\mathbf{r}, \mathbf{p}, t) \, d\mathbf{r} \, d\mathbf{p} = 1 \tag{34}$$

and

$$A(\mathbf{r}, \mathbf{p}, \mathbf{x}) = \sum_k a(\mathbf{R}^k, \mathbf{V}^k) \delta(\mathbf{R}^k - \mathbf{x}) \tag{35}$$

or

$$A(\mathbf{r}, \mathbf{p}, \mathbf{x}) = \sum_{k=1}^n \left(\sum_{\alpha=1}^v a^\alpha (\mathbf{R}^{k\alpha}, \mathbf{V}^{k\alpha}) \right) \delta(\mathbf{R}^k - \mathbf{x}). \tag{36}$$

This gives

(1) mass density

$$\bar{\rho} = \left\langle \sum_{k=1}^n m\delta(\mathbf{R}^k - \mathbf{x}) \middle/ \Delta V \right\rangle, \tag{37}$$

(2) linear momentum density

$$\bar{\rho}\bar{\mathbf{v}} = \left\langle \sum_{k=1}^n \mathbf{V}^k \delta(\mathbf{R}^k - \mathbf{x}) \middle/ \Delta V \right\rangle, \tag{38}$$

(3) microinertia density

$$\overline{\rho\mathbf{i}} = \left\langle \sum_{k=1}^n \sum_{\alpha=1}^v (m^\alpha \Delta\mathbf{r}^{k\alpha} \otimes \Delta\mathbf{r}^{k\alpha})\delta(\mathbf{R}^k - \mathbf{x}) \middle/ \Delta V \right\rangle, \tag{39}$$

(4) generalized spin density

$$\overline{\rho\boldsymbol{\phi}} = \left\langle \sum_{k=1}^n \sum_{\alpha=1}^v (m^\alpha \Delta\mathbf{v}^{k\alpha} \otimes \Delta\mathbf{r}^{k\alpha})\delta(\mathbf{R}^k - \mathbf{x}) \middle/ \Delta V \right\rangle, \tag{40}$$

(5) temperature

$$T = \frac{1}{3nvk} \left\langle \sum_{i=1}^n \sum_{\alpha=1}^v m(\mathbf{V}^{i\alpha} - \bar{\mathbf{v}} - \bar{\boldsymbol{\omega}}\Delta\mathbf{r}^{i\alpha})^2 \delta(\mathbf{R}^i - \mathbf{x}) \right\rangle, \tag{41}$$

(6) internal energy density

$$\bar{\rho}\bar{\varepsilon} = \left\langle \sum_{k=1}^n \left[\frac{1}{2}m(\mathbf{V}^k - \bar{\mathbf{v}})^2 + \sum_{\alpha=1}^v \left(\frac{1}{2}m^\alpha[(\boldsymbol{\omega}^k - \bar{\boldsymbol{\omega}}) \cdot \Delta\mathbf{r}^{k\alpha}]^2 + U^{k\alpha} \right) \right] \delta(\mathbf{R}^k - \mathbf{x}) \middle/ \Delta V \right\rangle, \tag{42}$$

(7) body force density

$$\bar{\mathbf{f}} \equiv \left\langle \sum_{k=1}^n \left(\sum_{\alpha=1}^v f_3^{k\alpha} \right) \delta(\mathbf{R}^k - \mathbf{x}) \middle/ \Delta V \right\rangle, \tag{43}$$

(8) body couple density

$$\bar{l} = \left\langle \sum_{k=1}^{n} \left(\sum_{\alpha=1}^{v} \boldsymbol{f}_3^{k\alpha} \otimes \Delta \boldsymbol{r}^{k\alpha} \right) \delta(\boldsymbol{R}^k - \boldsymbol{x}) \middle/ \Delta V \right\rangle. \tag{44}$$

The atomistic counterpart of stress is the flux of momentum (Hoover, 1986, 1991). From an atomistic viewpoint, there are two kinds of contributions to the flux of momentum, "kinetic" and "potential". The "kinetic" contribution comes from the flow of momentum due to atomic motion, $\boldsymbol{P}^{\mathrm{kin}} = \sum_i \boldsymbol{p}_i \otimes \boldsymbol{p}_i / m / \mathrm{d}V$. The "potential" flow of momentum, between all pairs of atoms within volume $\mathrm{d}V$ occurs through the mechanism of the interatomic forces; it is the transfer of momentum from atom i to atom j, $\boldsymbol{P}^{\mathrm{pot}} = \frac{1}{2} \sum_{i,j} \boldsymbol{R}_{ij} \otimes \boldsymbol{f}_{ij} / \mathrm{d}V$. There are three stresses in general Microcontinuum theory. From the viewpoint of the atomic model, the Cauchy stress is the stress evaluated at the center of the material particle; the microstress average is the stresses averaged over all atoms in the inner structure of the particle; and the moment stress, measuring the flux of the spin of the particle, results from the resultant moment of interatomic force within the inner structure of the particle.

By virtue of the possible macroscopic motion of the whole specimen, the velocity that makes contribution to stresses is $\boldsymbol{V}^k - \bar{\boldsymbol{v}}$, the difference between the instantaneous velocity and the stream velocity. Therefore we have

(9) Cauchy stress

$$\bar{\boldsymbol{t}}^{\mathrm{kin}} = -\left\langle \sum_{k=1}^{n} m(\boldsymbol{V}^k - \bar{\boldsymbol{v}}) \otimes (\boldsymbol{V}^k - \bar{\boldsymbol{v}}) \delta(\boldsymbol{R}^k - \boldsymbol{x}) \middle/ \Delta V \right\rangle, \tag{45}$$

$$\bar{\boldsymbol{t}}^{\mathrm{pot}} = -\left\langle \frac{1}{2} \int_0^1 \sum_{k,l=1}^{n} (\boldsymbol{R}^k - \boldsymbol{R}^l) \otimes \left(\sum_{\alpha,\beta=1}^{v} \boldsymbol{f}_1^{k\alpha}_{l\beta} \right) \delta(\boldsymbol{R}^k(1-\xi) + \boldsymbol{R}^l \xi - \boldsymbol{x}) \mathrm{d}\xi \middle/ \Delta V \right\rangle, \tag{46}$$

(10) microstress average

$$\bar{\boldsymbol{s}}^{\mathrm{kin}} = -\left\langle \sum_{k=1}^{n} \sum_{\alpha=1}^{v} m^{\alpha}(\boldsymbol{V}^{k\alpha} - (\bar{\boldsymbol{v}} + \bar{\boldsymbol{\omega}} \cdot \Delta \boldsymbol{r}^{k\alpha})) \otimes (\boldsymbol{V}^{k\alpha} - (\bar{\boldsymbol{v}} + \bar{\boldsymbol{\omega}} \cdot \Delta \boldsymbol{r}^{k\alpha})) \delta(\boldsymbol{R}^k - \boldsymbol{x}) \middle/ \Delta V \right\rangle, \tag{47}$$

$$\bar{\boldsymbol{s}}^{\mathrm{pot}} = -\left\langle \frac{1}{2} \int_0^1 \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{v} (\boldsymbol{R}^{k\alpha} - \boldsymbol{R}^{l\beta}) \otimes \boldsymbol{f}_1^{k\alpha}_{l\beta} \delta(\boldsymbol{R}^k(1-\xi) + \boldsymbol{R}^l \xi - \boldsymbol{x}) \mathrm{d}\xi \middle/ \Delta V \right\rangle$$
$$- \left\langle \frac{1}{2} \sum_{k=1}^{n} \left(\sum_{\alpha,\beta=1}^{v} (\boldsymbol{R}^{k\alpha} - \boldsymbol{R}^{k\beta}) \otimes \boldsymbol{f}_2^{k\alpha}_{\beta} \right) \delta(\boldsymbol{R}^k - \boldsymbol{x}) \middle/ \Delta V \right\rangle, \tag{48}$$

(11) moment stress

$$\bar{\boldsymbol{m}}^{\mathrm{kin}} = -\left\langle \sum_{k=1}^{n} (\boldsymbol{V}^k - \bar{\boldsymbol{v}}) \otimes (\boldsymbol{\omega}^k - \bar{\boldsymbol{\omega}}) \cdot \left(\sum_{\alpha=1}^{v} m^{\alpha} \Delta \boldsymbol{r}^{k\alpha} \otimes \Delta \boldsymbol{r}^{k\alpha} \right) \delta(\boldsymbol{R}^k - \boldsymbol{x}) \middle/ \Delta V \right\rangle, \tag{49}$$

$$\bar{\boldsymbol{m}}^{\mathrm{pot}} = -\left\langle \frac{1}{2} \int_0^1 \sum_{k,l=1}^{n} (\boldsymbol{R}^k - \boldsymbol{R}^l) \otimes \left\{ \sum_{\alpha,\beta=1}^{v} \boldsymbol{f}_1^{k\alpha}_{l\beta} \otimes [\Delta \boldsymbol{r}^{k\alpha}(1-\xi) + \Delta \boldsymbol{r}^{l\beta} \xi] \right\} \delta(\boldsymbol{R}^k(1-\xi) + \boldsymbol{R}^l \xi - \boldsymbol{x}) \mathrm{d}\xi \middle/ \Delta V \right\rangle. \tag{50}$$

(12) heat flux

Heat flux vector measures the conductive flow of energy per unit time and area. The flow of the energy, for all atoms in the volume dV, gives the kinetic contributions to the heat flux. It comes from the rate at which each particle carries energy with single-atom contribution: $q^{\text{kin}} = \sum p_i E/m/dV$. While the potential contributions to the heat flux occur whenever two moving atoms interact in such a way that one atom transfers a part of their joint energy to the other atom. It comes from the rate at which energy is transported through the action of interatomic forces: $q^{\text{pot}} = \frac{1}{2} \sum_{i,j} R_{ij}(p_i + p_j) \cdot f_{ij}/2m/dV$. This gives the averaged heat flux as

$$\bar{q}^{\text{kin}} = -\left\langle \sum_{k=1}^{n} (V^k - \bar{v}) \left[\frac{1}{2} m(V^k - \bar{v})^2 + \sum_{\alpha=1}^{v} \left(\frac{1}{2} m^\alpha [(\omega^k - \bar{\omega}) \cdot \Delta r^{k\alpha}]^2 + U^{k\alpha} \right) \right] \delta(R^k - x/\Delta V) \right\rangle, \qquad (51)$$

$$\bar{q}^{\text{pot}} = -\left\langle \frac{1}{2} \int_0^1 \sum_{k,l=1}^{n} (R^k - R^l) \sum_{\alpha,\beta=1}^{v} (V^{k\alpha} - \bar{v} - \bar{\omega} \cdot \Delta r^{k\alpha}) \cdot f_1^{\substack{k\alpha \\ l\beta}} \delta(R^k(1-\xi) + R^l\xi - x)\, d\xi/\Delta V \right\rangle. \qquad (52)$$

All the averaged field quantities come from the corresponding instantaneous forms that follow exactly the atomistic definitions. And the time evolution of conserved properties in the atomic model has been found to follow the same equations of balance laws in Micromorphic theory. For detailed formulation, readers are referred to the paper by Chen et al. (2003), Chen and Lee (2003b,c).

3.3. Applicability analysis of continuum theories from the viewpoint of molecular dynamics

3.3.1. Micromorphic theory

Atomistic flow mechanisms make it possible to define the fluxes as sums of one- and two-atom contributions. The internal energy ε, heat flux q, and the three stress tensors, namely, Cauchy stress t, microstress average s, and moment stress m, are composed of kinetic parts and potential parts. With the definition of temperature, the kinetic parts of t, s, m, q, and ε are caused by the thermal motion of atoms, and can be linked to the temperature. The potential parts are caused by the interatomic forces, and can be determined from the potential functions and written in terms of lattice strain and internal strains. This is consistent with the constitutive relations of Micromorphic theory. Therefore, Micromorphic theory, including the mechanical variables, balance laws, and constitutive relations, can be obtained based on the kinetics and interactions of atoms. The correspondence between the molecular dynamics model and the Micromorphic theory can be achieved whenever an ensemble average is meaningful. The applicability of Micromorphic theory in microscopic time and length scales is confirmed from the viewpoint of molecular dynamics.

3.3.2. Microstructure theory

In the case

$$T = \frac{1}{3nk} \sum_{i=1}^{n} m(V^i - \bar{v})^2 \to 0, \qquad (53)$$

which may be valid for the case of low temperature and small deformations. The kinetic parts of the stresses, t, s, m, the heat flux, q, and of the internal energy, ε, can be ignored. The expressions of t, s, m, q, and ε then reduce to Mindlin's microstructure theory of elasticity, and the balance laws still take the same form. This is the microscopic base of Microstructure theory. Hence, compared with Eringen's Micromorphic theory, Mindlin's microstructure theory holds for law temperature and small deformation problems.

3.3.3. Micropolar theory

If there is a very large difference between the atomic force $f_1^{k\alpha}{}_{l\beta}$ and $f_2^{k\alpha}{}_{k\beta}$, and $f_2^{k\alpha}{}_{k\beta}$ is much larger, the structure of the particle can then be approximated as rigid. Therefore, $\omega^k = \omega^k$, and $\Delta v^{k\alpha} = \omega^k \Delta r^{k\alpha}$. This then results in the Micropolar theory.

One typical example is molecular crystals, where the intramolecular bonds are essential first order bonds while the intermolecular bonds are generally second order, or in any case, considerably weaker than the former. Consequently the intramolecular binding energies are much higher and the intermolecular binding does not change significantly the structure of the molecule. As a consequence, the oscillation frequencies of the atoms within the molecules with respect to each other are much higher than the relative oscillation frequencies of the molecular groups. Hence the molecular groups can, to a reasonable approximation, be taken as rigid.

Apparently, this is not the case for metallic, covalent and ionic single crystals. Micropolar theory, therefore, can be applied in situations like molecular crystal, or materials that have rigid or near rigid microstructure. It is not suited for metallic, covalent and ionic single crystals.

3.3.4. Cosserat theory

Compared with Micropolar theory, Cosserat theory does not have the balance law of microinertia. The absence of the balance law of microinertia, implies that the microinertia tensor is assumed to be constant. This is the case when the deformation of the microstructure of the particle is very small, and the change of the orientation can be ignored. Hence, compared with Micropolar theory, Cosserat theory is not suited for problems involving the significant change of the orientation of the microstructure.

3.3.5. Nonlocal theory

For each atom (k, α), the interatomic force is taken from all other atoms in the body considered. These action-at-a-distance interactions give the related quantities a nonlocal character. Hence, the molecular dynamics formulation is in the nonlocal arena. Even in the limit case when the unit cell or the material particle only consists of one atom, the expressions and derivation are still applicable to nonlocal phenomena.

3.3.6. Couple stress theory

The couple stress theory, by including higher order stress, provides a model that can yield results depending on the size of specimen. However, there is no distinction between the micromotion and the macromotion, and hence this theory is suited only for material without microstructure.

Material that does not have microstructure is referred as microscopically homogeneous, and corresponds to crystal with only one atom in the unit cell. This follows that $m = m^\alpha$, $R^k = R^{k\alpha}$, $V^k = V^{k\alpha}$, and hence $s = t$ and the moment stress $m = 0$. The higher order stress, m, is thus removed from the atomic formulation. The couple stress theory then falls into the framework of nonlocal theory, with the strain gradients accounting for the effect of neighborhood.

4. Discussion

It is well-known that classical continuum theory predicts no optical vibration and no dispersive frequency–wave vector relations. Atomic models and classical continuum theory therefore cannot achieve a dynamic correspondence. A bridge is needed to fill the gap. This work has shown that the Micromorphic theory is able to encompass classical continuum theory at the macroscale and overlap a quite large region of atomic theories at microscale.

As the applications of microsystems multiply, various microcontinuum theories emerge. This work shows that if a continuum theory can achieve a correspondence with atomistic lattice dynamics and molecular dynamics, it is most likely in the framework of Micromorphic theory, nonlocal theory or the combination of both.

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