Examining the physical foundation of continuum theories from the viewpoint of phonon dispersion relation

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Abstract

An overview of crystal types and their interatomic force models are given and the basic feature of the dynamics of atoms in crystal is introduced. Elastic waves described by classical continuum theory, phonon dispersion relations by micromorphic theory, micropolar theory, couple stress theories and nonlocal theory are calculated and presented. The physical foundation and the applicability are examined from the viewpoint of phonon dispersion relation. Two physical examples, including the apparent change of material constants at different length scales and the macroscopic phenomenon of piezoelectricity are discussed.

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1. Introduction

Most of the solids with which physicists and materials scientists are concerned are crystalline. A large number of material features, such as material hardness, symmetry, chemical properties and electrical properties, can be explained on the basis of the atomic structure—the static atomic arrangement. There are, however, a lot of physical phenomena that can only be understood on the basis of atomic motion. Examples include the energy dissipation, temperature effects, specific heat, thermal expansion, thermal conductivity, phase transitions, piezoelectricity, melting, sound propagation, optical and dielectric properties, etc.
The dynamics of atoms in crystals—lattice dynamics—are thus very important to many fields of study in the solid state. It turned out to be most readily described not in terms of the individual atoms, but in terms of traveling waves, named lattice vibrations by Born [6], each characterized by a wave vector, a frequency, and certain polarization properties. These waves are the normal modes of vibration of the system. The frequency–wave vector relationship is called the phonon dispersion relation. The quantum of energy in an elastic wave is called a phonon. At a very low temperature a solid can be regarded as a volume containing non-interacting phonons. The vibrating lattice can be considered as a set of phonon excitations. Phonon dispersion relation is therefore an essential feature of atomic structure and atomic motion in crystal and is of special importance for solid state physics and material science.

The calculation of phonon dispersion relations, as a fundamental ingredient in the theory of lattice dynamics, has been studied by quantum mechanical methods or by phenomenological methods through interatomic force models. Either of them is able to yield very good results for a number of materials. The experimental measurements of phonon dispersion curves \( \omega(q) \) have played a very important role for studying phonons. By measuring the change in direction and in energy of the scattered neutrons, it is possible to obtain the whole phonon spectrum, i.e., phonon frequencies as a function of wave vectors for all the acoustic and optic branches. This phonon study has opened the possibility of obtaining detailed information about the interatomic forces and provided the chance of testing various potential models, and thus marked a new era in dynamics of crystal lattice.

The analog of atomic force is the constitutive relation in the continuum theory, which serves to distinguish one material from another. It follows that the phonon dispersion relations can also be calculated through the constitutive relations of a material by a continuum model if the model can manifest the dynamics of atoms in crystals. Therefore it provides a bridge to link the interatomic force to the constitutive relations. This also provides a chance for continuum field theories to be examined about their validity and applicability from the viewpoint of atomic structure and motions.

This paper aims to provide an atomistic viewpoint to examine the physical foundation of all the continuum theories through the well-known results of their frequency–wave vector relations. It is organized as follows: in Section 2 an overview of the crystal types and the interatomic force model is given; in Section 3 the basic feature of phonon dispersion relations is introduced; the elastic waves by classical continuum theory, phonon dispersion relations by micromorphic theory, by micropolar theory, by couple stress theories and by nonlocal theory are calculated or cited and presented in Sections 4–8, respectively; the physical foundation and the applicability are examined through crystal dynamics; the paper ends with some discussions and two examples in Section 9.

2. An overview on crystal types and interatomic force models

2.1. Solid inert gases

The choice of the interatomic force model depends on the type of binding between the atoms. For the solid inert gases, a good model is based on the Leonard–Jones potential that describes the weak van der Waals attractive forces and the repulsive forces between pairs of neutral atoms. For
In metals the atomic cores (nuclei plus the tightly bound inner electrons) are surrounded by a more-or-less uniform density of free electrons. It is this general distribution of electrons that gives metals their electrical conductivity. The role of those free electrons is to screen out the Coulomb interaction between the positive ions, thereby stabilizing the lattice and reducing considerably the range of interatomic forces. A substantial number of metals have been measured using neutron scattering technique [8,9,38,39]. There have been calculations by the pseudopotential method [31,32], the force constant model [10], and the embedded atom method [34]. It has been repeatedly stressed that the model potential or true pseudopotential is nonlocal and the nonlocality should be retained in an accurate calculation [5,30,47,52].

2.3. Ionic crystal

In ionic crystals, strong Coulomb forces and short-range repulsive forces operate between the ions. The rigid-ion model, in which the ionic charges are approximated by point charges centered at the nuclei, describes both the long-range Coulomb interactions and the short-range interactions [10]. In reality, however, the ions are not rigid but polarizable. In the course of a lattice vibration, the electric field set up by the displacement of the ions is modified by the electronic polarizability, and this modifies the forces and affects the phonon frequencies. The shell model [15] was developed for ionic crystal with polarizable ions, in which an atom is represented by a non-polarizable ion core and a shell of valence electrons. The displacement of the shell relative to the core produces a dipole. An ion core and its shell are regarded as point charges when dealing with the Coulomb interaction with other ion cores and shells. In the simplest shell model a minimum of five independent parameters are needed to describe core–core, core–shell and shell–shell forces extending to the nearest neighbor, up to 14 parameters are needed for better fit of experimental measurements. An extension of the shell model is the deformable shell model or breathing shell model proposed by Schroder [49] and Kress [35]. Ab initio calculations, by the direct method, for alkaline-earth oxides, such as MgO, CaO, SrO, can be found in [43,50].

2.4. Covalent crystal

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. For covalent crystals such as diamond, silicon or germanium, it has been found in practice that the shell model with 14 parameters gave quite good agreement with the experimental measurements ([16,54]). This success underlies some similarity between ionic and covalent solids. The bond charge model [46,55] could be regarded as an extension of the shell model for covalently bonded atoms. Four types of interactions are considered in the adiabatic bond charge model: (i) Coulomb interaction between ions and bond charges: (ii) nearest-neighbor ion–ion central interaction: (iii) ion–bond charge central interaction, and (iv) bond charge–bond...
charge non-central (or bond-bending) interaction. This model has been applied to the study of lattice dynamics of diamond and zincblende type semiconductors with four and six parameters respectively and yielded very good results compared to the experimental measurements [46]. Another model can be used for covalent or partially covalent crystal is the valence force model, which has originally been developed for vibrations in molecules. The potential energy is expressed in terms of changes in bond distances and bond angles and involves six independent force constants [10]. Also, ab initio calculations are available in literature [4,56].

2.5. Molecular crystal

One of the main features of molecular crystal is that there is usually a large difference between the frequencies of modes in which the molecules move as rigid units (the external modes) and the modes which involve the stretching and distortion of the molecules (the internal modes). The external modes usually have frequencies below 3–4 THz, whereas the internal mode frequencies will be an order of magnitude higher and usually have only a weak dependence on wave vector [19]. For molecular crystals or crystals containing complex ions, it is often possible to separate the internal vibrations within the molecules from their external vibrations and to simplify the model by identifying the well-bound molecules or complex ions in the crystal and treating them as rigid bodies [10,17,18,57]. These rigid bodies execute both translational and rotational oscillations, giving six degrees of freedom per molecule. The effects of non-rigidity of the molecules or complex ions may be examined separately.

2.6. Framework crystal

Many materials contain or consist of rather rigid units such as tetrahedral, octahedral or planar triangles. In what is termed framework structure crystal these form a continuous network by sharing corner atoms between adjacent units. Examples are many alumino-silicate containing AlO₄ and SiO₄ tetrahedral and perovskites containing XO₆ octahedral. The basic feature of framework structure is that the units are very stiff but linked flexibly to each other at the corner atoms. The framework crystals are in many respects similar to molecular crystals in that they are composed of rigid groups. The characteristics of their phonon dispersion relations is the soft modes, which also called “rigid unit modes”, that can propagate with no distortion of the units. Rigid unit modes have been found to be particularly important in silicates [51]. Theoretical calculations of the interactions in silicate have been carried out by using the quantum mechanics of small clusters [36,37,42]. It turns out that silicate minerals can be modeled surprisingly accurately by using simple model interaction for Si–O and O–O interactions, bond-bending O–Si–O interaction to account for the covalent nature of the Si bonding, and a shell model for the oxygen atoms to account for the relatively high polarizability of the O²⁻ ion [48].

3. Basic feature of phonon dispersion relations

Phonon frequencies are the eigenvalues of a dynamical matrix. For a unit cell, k, with v atoms, the equation of motion can be obtained as
\[ \omega^2(q)m_k \alpha U_i(\alpha, q) = \sum_{\beta=1}^{3} \sum_{j=1}^{3} D_{ij}(\alpha \beta, q) U_j(\beta, q), \]  

(3.1)

where \( \omega \) is the frequency, \( q \) the wave vector, and \( D \) is called the dynamical matrix. The condition for the equation to have non-trivial solution is

\[ \det(D - m\omega^2) = 0. \]  

(3.2)

There are \( 3n \) solutions for \( \omega \) for each \( q \) in above equation, written as \( \omega_j(q), j = 1, 2, \ldots, 3n \), and the corresponding wave-amplitudes or polarization vectors \( U(k, q, j) \). In a primitive basis of two identical silicon atoms, the phonon dispersion relations calculated by different methods are shown in Fig. 1 in which the transverse branches are double. The typical motions are shown in Fig. 2.

Generally, in the limit \( q \to 0 \), the acoustic modes have all the atoms moving in phase, whereas the optical modes have the atoms moving out of phase [19]. Optical branches are vibration modes within the unit cell. For a unit cell containing \( n \) atoms there will be 3 acoustic branches and \( 3n - 3 \)

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**Fig. 1.** Phonon dispersion relations for silicon. Solid line: shell model (after [12]); dot line: ab initio (after [56]); symbols: experimental measurement (cf. [12]).

**Fig. 2.** Typical motions for the two atoms in the unit cell.
For a unit cell with \( m \) molecules and with \( f \) atoms per molecule, there will be 3 acoustic modes and \( 3mf - 3 \) optical modes, of which \( 3m(f - 2) \) will be the internal modes.

The frequencies in the acoustic branches are audible, for this reason these branches are called “acoustic”. The frequencies in the optical branches are typically in the infrared, close to the optical frequencies, and so those branches are called “optical”. Under an electromagnetic field it is the optical modes that are excited. Optics is a phenomenon that necessitates the presence of an electromagnetic field. The long-wavelength acoustic vibration is the physical foundation of classical continuum theory modes have a connection with the elastic properties. While, while the optical vibration is the mechanism of a lot of macroscopic phenomena involving thermal, mechanical, electrical and optical coupling effects.

In an optical vibration of non-central ionic crystal, atoms of one type move as a body against the atoms of the other type. The relative displacement between the positive and negative ions gives rise to the macroscopic phenomenon: piezoelectricity. The energy of a crystal involves both the acoustic and optical vibrations. Differentiating energy with respect to temperature yields the macroscopic property: specific heat. Application of a temperature gradient across a solid excites the elementary excitations, such as free electrons, holes and phonons, that conduct heat from the hotter to the colder end of the specimen. In metals both electrons and phonons play their role. In dielectrics or intrinsic semiconductors almost all heat is conducted by phonons (heat conduction). Also, phonon scattering mechanisms give rise to thermal resistance (i.e., a finite thermal conductivity). In the language of continuum physics, it is seen that phonon is a base to understand the coupling effect between thermal, mechanical, electrical, and optical properties.

Optical vibrations of long wavelengths are of special importance in considering those coupling effect. In general an electromagnetic wave interacts only with lattice vibrations of the same wavelength, and will be strongly affected only if its frequency is near that of the latter. The frequencies of lattice vibrations are generally in the range from 0 to \( 10^{13}/s \). Light waves of similar frequencies have wavelengths larger than \( c \times 10^{-13} = 0.003 \) cm \( (c \) is the speed of light), which are enormously large compared with the lattice constants of crystal. So, the lattice vibrations that can interact appreciably with light are very long waves. Also, it is in the long wavelength optical vibrations, the opposed motions of the oppositely charged particles give rise to a net oscillating dipole moment of a cell. Therefore in the discussion of the coupling between mechanical, electromagnetic and optical behaviors of crystals only the long waves of the optical branch will concern us.

4. Elastic waves by classical continuum theory

Classic continuum mechanics views the crystal as a homogeneous continuous medium rather than a periodic array of atoms. The lattice particles are taken without structure and are idealized as point masses. In continuum theory the equation of motion of a crystal can be written, in tensor notation, as

\[
\rho \ddot{u}_i = \sigma_{ij,j},
\]

and under small deformation assumption, the stresses are linear functions of strains and the strains are first order derivatives of displacements:
\[ \sigma_{ij} = C_{ijkl} e_{kl}, \] (4.2)
\[ e_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}), \] (4.3)

where \( \rho \) is the density, \( \sigma_{ij} \) are the stresses, \( e_{ij} \) are the strains, \( u_i \) is the \( i \)th component of the displacement vector, respectively, and \( C_{ijkl} \) are the elastic constants. For a cubic crystal the elastic matrix reduces to a matrix with only three independent constants, i.e., \( C_{11}, C_{12}, C_{44} \).

Assuming a harmonic wave propagating along \( x \) direction
\[ u_i = U_i \exp [i(kx - \omega t)], \] (4.4)

it is easy to find
\[ \omega_L^2 = C_{11} k^2 / \rho, \] (4.5)
\[ \omega_T^2 = C_{44} k^2 / \rho. \] (4.6)

Those are acoustic waves. The frequency–wave vector relations are shown in Fig. 3. So, classical continuum theory yields non-dispersive frequency–wave vector relationship and acoustic branches only. They can be identical to the very long-wavelength solution of acoustic vibrations of atoms. The frequency region for which the continuum approximation is valid is of importance in solid state physics. Ultrasonic waves are used to measure elastic constants and to study the lattice defects, electronic structure of metals, and superconductivity [33]. There are also numerous technological applications of elastic waves in solid.

The classical continuum theory is the long acoustic wave limit of lattice dynamics [3]. So, the continuum approximation is only valid for elastic waves of very long wavelengths, corresponding to large length and time scales, and predicts properties independent of specimen size. For physics involving optical vibrations, or for problems in the small length and time scales where the dynamics of atoms become too important to be neglected, classical continuum mechanics would break down and fail to give good explanations.

Fig. 3. Elastic waves by classical continuum theory.
5. Micromorphic continuum theory and the phonon dispersion relations

In Eringen’s [20,24] microcontinuum field theory, also called micromorphic continuum theory, a material body is envisioned as a collection of a large number of deformable particles, each particle possesses finite size and directions representing its microstructure. The particle has the nine independent degrees of freedom describing both stretches and rotations, in addition to the three classical translational degrees of freedom of its center, and may be considered as a polyatomic molecule, a primitive unit cell of a crystalline solid, or a chopped fiber in a composite, etc.

The equations of motion for micromorphic material can be written as

\[ t_{kl,k} + \rho (f_l - \dot{v}_l) = 0, \]  

(5.1)

\[ m_{klm,k} + t_{ml} - s_{ml} + \rho (l_{lm} - \phi_{lm}) = 0, \]  

(5.2)

and under the assumption of small strain, slow motion, spin isotropy, and in the absence of body force and body couple, the equations of motion become

\[ t_{kl,k} = \rho \ddot{u}_l, \]  

(5.3)

\[ m_{klm,k} + t_{ml} - s_{ml} = \rho \ddot{j}_\phi_{lm}, \]  

(5.4)

where \( f \) is body force, \( l \) the body couple, \( \phi \) is the spin inertia; \( t \) is the Cauchy stress, \( m \) the moment stress, and \( s \) the microstress average; \( \rho \) is the mass density, \( i \) the microinertia, \( u \) and \( j \) are macro- and micromotion, respectively. In such a case, the strains are related to the displacements and micromotions as

\[ \gamma_{ij} = u_{j,i} - \phi_{ji}, \]  

(5.5)

\[ \eta_{ij} = \eta_{ji} = \frac{1}{2} (\phi_{ij} + \phi_{ji}), \]  

(5.6)

\[ \lambda_{ijk} = \phi_{jk,i}, \]  

(5.7)

and the stresses can be obtained as

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

(5.8)

\[ m_{ijk} = c_{ijklmn} \lambda_{mn}, \]

\[ = c_1 \delta_{ij} \lambda_{kmn} + c_2 \delta_{ij} \lambda_{knm} + c_3 \delta_{ij} \lambda_{mkn} + c_4 \delta_{ik} \lambda_{jmn} + c_5 \delta_{ik} \lambda_{jm} + c_6 \delta_{ik} \lambda_{mnj} + c_7 \delta_{jk} \lambda_{imm} + c_8 \lambda_{ijk} + c_9 \lambda_{ikj} + c_{10} \lambda_{jik} + c_{11} \lambda_{jki} + c_{12} \lambda_{jkl} + c_{13} \lambda_{jlk} + c_{14} \lambda_{jkl}, \]  

(5.9)

\[ s_{ij} = b_{ijkl} \eta_{kl} + d_{ijkl} \gamma_{kl} = b_1 \delta_{ij} \eta_{kk} + b_2 (\eta_{ij} + \eta_{ji}) + d_1 \delta_{ij} \gamma_{kk} + d_2 (\gamma_{ij} + \gamma_{ji}). \]  

(5.10)

For isotropic elastic solid the above stress–strain relations involves 14 elastic constants ([11]). Assuming harmonic waves propagating along the \( x \)-direction as
\[ u_i = i U_i e^{i(kx - \omega t)}, \quad (5.11) \]

\[ \Phi_{ij} = \Phi_{ij} e^{i(kx - \omega t)}, \quad (5.12) \]

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

1. **LRO (longitudinal external rotational optical wave)**

\[(Ak^2 + B - \rho \omega^2)\Phi_{[23]} = 0, \quad (5.13)\]

2. **TSO (transverse internal shear optical waves)**

\[(\bar{A}k^2 + \bar{B} - \rho \omega^2)(\Phi_{(23)}; \Phi_{22} - \Phi_{33}) = 0, \quad (5.14)\]

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

\[
\begin{vmatrix}
A_{11}k^2 - \rho \omega^2 & A_{12}k & A_{13}k \\
A_{12}k & A_{22}k^2 + B_{22} - \frac{3}{2} \rho \omega^2 & A_{23}k^2 \\
A_{13}k & A_{23}k^2 & A_{33}k^2 + B_{33} - 3\rho \omega^2
\end{vmatrix}
\begin{bmatrix}
U_1 \\
\Phi'_d
\end{bmatrix} = 0, \quad (5.15)
\]

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

\[
\begin{vmatrix}
\bar{A}_{11}k^2 - \rho \omega^2 & \bar{A}_{12}k & \bar{A}_{13}k \\
\bar{A}_{12}k & \bar{A}_{22}k^2 + \bar{B}_{22} - 2\rho \omega^2 & \bar{A}_{23}k^2 \\
\bar{A}_{13}k & \bar{A}_{23}k^2 & \bar{A}_{33}k^2 + \bar{B}_{33} - 2\rho \omega^2
\end{vmatrix}
\begin{bmatrix}
U_2 \\
U_3 \\
\Phi_{(12)} \\
\Phi_{(13)}
\end{bmatrix} = 0, \quad (5.16)
\]

where

\[ \Phi_{(ij)} \equiv \frac{1}{2} (\Phi_{ij} + \Phi_{ji}), \quad (5.17) \]

\[ \Phi_{(ij)}' \equiv \frac{1}{2} (\Phi_{ij} - \Phi_{ji}), \quad (5.18) \]

\[ \Phi \equiv \frac{1}{3} (\Phi_{11} + \Phi_{22} + \Phi_{33}), \quad (5.19) \]

\[ \Phi_{11}'' \equiv \Phi_{11} - \Phi. \quad (5.20) \]

These dispersion relations involve all the 14 elastic constants in the micromorphic elasticity. The solution of above equations can be sketched as in Fig. 4.

It is seen that the micromorphic continuum theory of order 1 can provide up to 12 dispersion relations, including three acoustic, nine optical. Among them there are six internal modes and
six external modes. Both the atomic structure and the dynamics of atoms have been manifested in micromorphic theory. For a material with several thousands to millions atoms, when an ensemble average is meaningful, continuum treatment will still be effective ([11]). According to the overview of crystal types mentioned in Section 2, it is expected that the micromorphic theory can give good and efficient descriptions for the dynamics of atoms in the following crystals:

1. covalent and ionic crystal in which the presence of both acoustic and internal optical vibrations is important;
2. molecular crystal, complex ionic or covalent crystal, and framework crystals, in which both internal and external modes exist.

Atomic models based on phenomenological theory can give a good fit to the experimentally measured phonon frequencies. It has been reported that a model with up to 15 parameters may be required [12,44,45], and these parameters do not contain conceptual simplicity. That is one reason why a priori quantum mechanical calculation of phonon spectra was needed and developed. On the other hand, microcontinuum theory treats the material as a continuum with 12 degrees for each particle and up to 14 material constants for isotropic elastic materials and hence dramatically enlarges the region of applicability, and nevertheless it can describe the essential feature of the dynamics of atoms and give good fit to the experimental measurements.

The theory of microstructure in linear elasticity, developed by Mindlin [40], is a subcase of Eringen’s micromorphic theory. Upon the assumptions of small deformation, slow motion, constant microinertia, spin isotropy and linear isotropic elasticity, the micromorphic theory can be reduced to the microstructure theory. Recalling the derivation of phonon dispersion relations of micromorphic solid, it can be seen that Mindlin’s microstructure theory can yield similar phonon dispersion relations. However, those assumptions lead to a limitation in its applications related to atomic motions, such as the thermal mechanical coupling, phase transition, anisotropic and large deformation problems.
6. Micropolar theory and the phonon dispersion relations

When the material particle is considered as rigid, the micromorphic theory is reduced to micropolar theory [20]. Each particle has three independent degrees of freedom for microrotations in addition to the 3 classical translational degrees of freedom of the center. In the absence of body force and body couple, and under assumptions of small strain, slow motion and microisotropy, the equations of motion for micropolar materials can be written as

\[ \sigma_{ij,j} = \rho \ddot{u}_j, \]  
\[ m_{ij,i} + \epsilon_{jkl} \sigma_{kl} = \rho j \ddot{\phi}_j, \]

and the constitutive relations can be obtained as

\[ \sigma_{ij} = A_{ijkl} e_{kl}, \]
\[ m_{ij} = B_{ijkl} \tau_{kl}, \]

where

\[ e_{kl} = u_{l,k} + e_{lkmm} \phi_m, \]
\[ \tau_{kl} = \phi_{l,k}. \]

For isotropic material, the equations of motion become

\[ \lambda u_{i,ij} + \mu_1 u_{j,ii} + \mu_2 u_{i,ij} - (\mu_1 - \mu_2) e_{ijk} \phi_{k,i} = \rho \ddot{u}_j, \]
\[ (\lambda + \mu_2) \phi_{i,ij} + \mu_1 \phi_{j,ii} - (\mu_1 - \mu_2) (e_{jkl} u_{k,l} + 2 \phi_j) = \rho j \ddot{\phi}_j. \]

Assuming harmonic waves

\[ u_i(x, t) = U_i e^{i(kx - \omega t)}, \]
\[ \phi_i(x, t) = i \Phi_i e^{i(kx - \omega t)}, \]

the following dispersion relations can be obtained:

1. LA (longitudinal acoustic wave)

\[ \begin{cases} u_x = U_1 e^{i(kx - \omega t)}, \\ \dot{u}_y = \dot{u}_z = \dot{\phi}_x = \dot{\phi}_y = \dot{\phi}_z = 0, \end{cases} \]
\[ (\lambda + \mu_1 + \mu_2) k^2 = \rho \omega^2, \]
(2) LRO (longitudinal rotational optical wave)

\[
\begin{aligned}
\phi_1 &= i\Phi_1 e^{i(kx - \omega t)}, \\
u_x &= u_y = u_z = \phi_y = \phi_z = 0, \\
(\lambda + \mu_1 + \mu_2)k^2 + 2(\mu_1 - \mu_2) &= \rho j\omega^2 \\
\end{aligned}
\]

(6.13)

with a cut-off frequency

\[
\omega_c = \sqrt{\frac{2(\mu_1 - \mu_2)}{\rho j}},
\]

(6.14)

(3) TA, TRO (transverse acoustic and transverse rotational optical waves)

\[
\begin{aligned}
u_y &= U_2 e^{i(kx - \omega t)}, \\
\phi_2 &= i\Phi_3 e^{i(kx - \omega t)}, \\
\phi_x &= \phi_y = 0, \\
\rho^2 j\omega^4 - \rho \omega^2 \{k^2(\mu_1 + \mu_2) + 2(\mu_1 - \mu_2)\} + \mu_1 \mu_1 k^4 + (\mu_1 + \mu_2)(\mu_1 - \mu_2)k^2 &= 0
\end{aligned}
\]

(6.15)

(6.16)

with a cut-off frequency

\[
\omega_c = \sqrt{\frac{2(\mu_1 - \mu_2)}{\rho j}}.
\]

(6.17)

The similar results can be obtained for the transverse waves with

\[
\begin{aligned}
u_z &= U_3 e^{i(kx - \omega t)}, \\
\phi_y &= i\Phi_2 e^{i(kx - \omega t)}, \\
\phi_x &= \phi_z = 0.
\end{aligned}
\]

(6.18)

(6.19)

Hence, micropolar theory yields the dispersion relations with six external modes only, as shown in Fig. 5. They include the longitudinal and transverse acoustic branches, and the rotational optical waves.

Fig. 5. Dispersion relation curves calculated by micropolar theory.
branches. They are the translational and rotational vibrations of rigid units, respectively. The optical modes (LRO and TRO) are identical to those “soft optical modes” observed in many framework crystals [51], ferroelectric crystals [3,12]. For molecular crystals, crystals containing complex ions, or complex covalent crystal, or framework crystal, or for chopped composite, granular material et al, 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 to the dynamics of microstructure. It accounts for the effect of both atomic structure and the dynamics of atoms.

Micropolar theory requires only six degrees of freedom per particle, and for isotropic material it just has six material constants. Nevertheless it stems from the consideration of microstructure and micromotions, and is expected to be effective for physical phenomena involving microscopic time and length scales for molecular crystal, some complex ionic or covalent crystal, framework crystal, chopped composite, granular material, etc.

Cosserat theory [13] is a special case of micropolar theory, where the balance law of microinertia is missing. The evolution of the inertia tensor with motion determines the anisotropic character of a body at any time. Phase transitions and displacive phase transition, as in those ferroelectric crystals, are the results of the change of the microinertia tensor with temperature. Cosserat continuum could yield similar phonon dispersion relations, however, the applicability would be restricted to problems involving large deformation or high temperature, for which a conservation law for microinertia tensor is needed.isotropic material and certain physical phenomena.

7. Couple stress theory and the dispersion relations

Couple stress theory [41,53], by including high order stresses, provided a model that can support body and surface couples. In the absence of body force and body couple, the linear equations of motion can be expressed as

\[ -m_{ijk,ij} + t_{ik,i} = \rho \ddot{u}_k - \frac{1}{3} \left( \rho' \dot{d}_{ij}^2 \ddot{u}_k,i, \right). \]  

(7.1)

The constitutive relations for isotropic materials take the form

\[ t_{ij} = \lambda \epsilon_{ij} + 2\mu \epsilon_{ij}, \]  

(7.2)

\[ m_{ijk} = \frac{1}{2} a_1 (u_{i,mm} \delta_{jk} + 2u_{m,nk} \delta_{ij} + u_{j,mm} \delta_{ik}) + a_2 (u_{m,mi} \delta_{jk} + u_{m,mj} \delta_{ik}) + 2a_3 u_{k,mm} \delta_{ij} + 2a_4 u_{k,ij} + a_5 (u_{i,jk} + u_{j,ik}). \]  

(7.3)

Assuming harmonic waves

\[ u_i(x,t) = U_i e^{i(kx-\omega t)} \]  

(7.4)

there results the LA and TA dispersion relations
Both are dispersive, but as \( k \to 0, \omega \to 0 \). They are acoustic waves only. The strain gradient theory \([25,26]\) falls within the framework of couple stress theory, and its dynamic generalization will yield the same acoustic dispersion relation.

There is also another strain gradient plasticity that incorporates a Laplacian strain \([1,2]\). The wave equation for one-dimensional gradient-dependent plasticity theory was derived by de Borst et al. \([14]\) as

\[
\frac{g}{h + E} \left[ E \frac{\partial^4 u}{\partial x^4} - \rho \frac{\partial^4 u}{\partial x^2 \partial t^2} \right] + \rho \frac{\partial^2 u}{\partial t^2} - \frac{hE}{h + E} \frac{\partial^2 u}{\partial x^2} = 0. \tag{7.7}
\]

For a single harmonic wave which propagates through one-dimensional element

\[
u(x,t) = U \exp[i(kx - \omega t)], \tag{7.8}
\]

the dispersion relation could be elaborated as

\[
\omega = k \sqrt{\frac{E}{h + gk^2}} \sqrt{\frac{h + gk^2}{E + h + gk^2}}, \tag{7.9}
\]

where \( h \) is the hardening/softening modulus, \( E \) the Young modulus, \( g \) a coefficient in the Taylor series expansion of the yield function. This yields a nonlinear dispersion relation with a cut-off value for \( k \), but is only an acoustic branch.

It is seen that the couple stress theory as well as the strain gradient theories incorporate higher order stresses, can support body and surface couples and so yield some properties related to the size of specimen. However, in these theories, there is no distinction between macromotion and micromotion, no optical vibrations can be described, and did not stem from the consideration of microstructure or micromotion.

### 8. Nonlocal theory and dispersion relations

Generally any problem that requires the solution of integro-differential equations can be said to be nonlocal in character. In a lattice structure of crystal, the interatomic forces acting on an atom depend on the relative atomic distances between this atom and its neighboring atoms. In the language of continuum mechanics, this is equivalent to the statement that the stresses at a point \( x \) are functions of the strains at all points of the body as expressed in

\[
\sigma_{ij}(x) = C_{ijkl}e_{kl}(x) + \int c_{ijkl}(x, x')e_{kl}(x') \, dx'. \tag{8.1}
\]
The strain gradients appear after the performance of the integrations when $\varepsilon_{kl}(x')$ is written as a Taylor series around point $x$.

For isotropic material, the phonon dispersion relations based on a nonlocal theory have been obtained by Eringen [23] as shown in Fig. 6. Remarkable similarity to atomic lattice dynamics solution with Born–von Karman model, and to the experimental results for Aluminum has been reported.

Nonlocal theory takes long-range interatomic interaction into consideration. As a consequence it 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. The solution of phonon dispersion relations shows that the nonlocal theory is only applicable for crystal that only has one atom per primitive unit cell. Metallic crystal is the promising material for the application of nonlocal theory. Both micromorphic theory and nonlocal theory will benefit from their incorporation, which will provide the great chance for microcontinuum physics to be applied to nano scale problems.

Although the strain-gradient theory is an improvement from the local theory and as such may account for some limited nonlocality, it cannot, however, be equated to the nonlocal continuum theory of Eringen [22], which offers the best description of physical phenomena at the micro- and nanoscales besides serving the usual marcodomain in the classical limit.

9. Discussions

9.1. The promise of micromorphic continuum theory

The entire physical science is based on two fundamental physical models: (1) discrete atomistic models, (2) continuum field theories. An elementary but crucial criterion that clearly provides an acid test for the limitations of either one of the two models is the ratio of characteristic length (or time). The success of a theory depends on the ratio of a characteristic length $l$ (or time $\tau$) inherent to the inner structure of bodies to the characteristic length $L$ (or time $T$) of the disturbance. For large length (or time) scale, $l/L \ll 1$ (or $\tau/T \ll 1$), the subbodies (atoms, molecules, or grains) act collaboratively so that the statistical averages are meaningful and hence a good continuum theory is successful, while a discrete model is not practical and unnecessary. On the other hand, for small
length (or time) scale problem, \( l/L \rightarrow 1 \) (or \( \tau/T \rightarrow 1 \)), the individual subbodies respond to the external effect more or less independently, so that continuum approximations fail to hold and one must resort to a discrete model [21].

It is seen that the micromorphic continuum theory shares the essential feature of the discrete atomic lattice dynamics and can describe the effects of both atomic structure and atomic motion, and hence has dramatically extended the continuum field theories down towards microscopic length and time scales and towards microscopic physics. For an \( N \)-body system, as long as the ensemble average can describe the behaviors of the system so that the continuum treatment is valid [28], the micromorphic theory can assume an honorable place on par with the atomic model for both the power and practicality.

Also, from the viewpoint of phonon dispersion relations, it is seen that the micromorphic theory was built on the foundation of lattice dynamics, and the continuum treatment has enlarged the application field of lattice dynamics to a much larger length (or time) scale and to macroscopic physics.

While polar theories (micromorphic and micropolar) appear to be effective in the range down to \( l = 10^3 \) angstrom. Below this limit, for perfect lattices, it is necessary to construct theories that encompass long-range atomic interactions [21,58]. Therefore incorporating the polar theories with the nonlocal theory [22] will provide the chance for continuum field theory to go further top–down from microlevel to nanolevel.

9.2. The lattice dynamics foundation of micropolar theory

Molecular crystals are made of groups of atoms and the bindings are of two different types: intramolecular and intermolecular, which are responsible for atoms to form an isolated molecule and for molecules to form the crystal, respectively. 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 [3]. Consequently the intramolecular binding energies are much higher and the intermolecular binding does not change significantly the structure of the molecule. Furthermore, as a consequence of strong intramolecular bonds, 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 [19]. These considerations imply that for the lattice model, which are the relative motions of the molecular groups, the frequencies are sufficiently low and do not excite intramolecular motions. Hence the molecular groups can, to a reasonable approximation, be taken as rigid.

The framework structure crystals, which have great potential for applications such as piezoelectric applications, are in many respects similar to molecular crystals in that they are composed of rigid groups, but they are different in that the units are linked flexibly to each other at the corner atoms. So, does framework have any geometrically allowed phonon modes of motion in which the units only rotate and/or translate as rigid wholes? The answer is that such “rigid unit modes” do indeed exist along special directions in Brillouin zone [29]. Clearly, in a real material, the rigid unit modes will be phonons with a relatively low frequency with perhaps one of them resulting in a soft-mode phase transition, while all other phonons are typified by much higher frequencies because they necessarily involve distorting the rather stiff units.
Those physics of molecular crystal and framework crystal naturally lead to a model of a lattice where the particles are considered to be of finite size and rigid, and thus the lattice particles are characterized not only by a mass but also a microinertia. It then follows that the dynamics can be defined not only by the displacement of the particles, but also by their rotation. Obviously, the equilibrium configuration is defined together by the positions and orientations of particles for minimizing the energy of deformation. This is the physical picture of the micropolar theory. In the micropolar theory, the particle possesses finite size and orientation which representing the microstructure and describing their micromotion.

The lattice dynamics foundation of micropolar theory is the dynamics of molecular crystal, dynamics of framework crystal, dynamics of soft-mode phase transitions. Its application region includes molecular crystals, some complex ionic and covalent crystals, framework crystals, and materials that are not crystals but have rigid or nearly rigid microstructures, such as granular materials, chopped composites, etc.

9.3. The optical branch and the limitations of other continuum theories

As mentioned before, under an electromagnetic field it is the optical modes that are excited. Optics is a phenomenon that necessitates the presence of an electromagnetic field. Optical vibration is the mechanism of a lot of macroscopic phenomena involving thermal, electrical, mechanical and optical coupling properties, e.g. piezoelectricity, heat conduction, thermal conductivity, thermal resistance, and melting, etc. Optical modes are either the vibrational modes within a unit cell or the rotational model of a united group. Its presence represents the microstructure and the micromotion.

The absence of optical branch is due to the neglecting of the atomic structure of crystal. From this viewpoint, classical continuum theory, the gradient theories, and the couple stress theories do not stem from the considerations of microstructure or micromotion and as a consequence, would break down if the micromotion and/or the microstructure become too significant to be neglected.

9.4. Two physical examples

As the applications of microsystem and microelectromechanical system increase, a lot of phenomena have emerged, for which it is found that classical continuum theory is no long valid. Two of the examples are:

9.4.1. The change of material constants as the size goes down to micron or submicron

Size effect is now well accepted. One of the size effects that has been repeatedly reported is the elastic moduli, such as Young's modulus, change as the size changes from macroscopic to microscopic. However, from the viewpoint of lattice dynamics, elastic constants in classical continuum mechanics can be completely and uniquely determined by phonon dispersion relations using the long acoustic wave limit method ([7,12]). For example, the nearest atomic interaction in Born–von Karman interatomic force model for diamond structure crystal yields a dynamical matrix
\[ D = \begin{bmatrix} 4a & 0 & 0 & -4aC_x & 0 & 0 \\ 0 & 4a & 0 & 0 & -4aC_x & 4ibS_x \\ 0 & 0 & 4a & 0 & 4ibS_x & 4aC_x \\ 4a & 0 & 0 & \text{(complex)} & 0 & 4a \\ \text{conjugate)} & 0 & 4a & 0 & \text{4a} \end{bmatrix}, \] (9.1)

where \( C_i = \cos \frac{1}{2} q_i r_0 \), \( S_i = \sin \frac{1}{2} q_i r_0 \), \( i = x, y, z \), \( a \) and \( b \) are atomic force constants, \(-\phi_{ij}(k\alpha, l\beta)\), in the following equations of force–displacement relations:

\[ F(k\alpha) = -\Phi(k\alpha, l\beta)u(l\beta), \] (9.2)

\[ -\Phi(k1, k2) = \begin{pmatrix} a & b & b \\ b & a & b \\ b & b & a \end{pmatrix}. \] (9.3)

The eigenvalues of the dynamical matrix give the phonon frequencies and the eigenvectors give the vibrational modes of phonons. By considering the acoustic modes and taking the limit of \( \omega/q \) as \( q \to 0 \) one finds that the elastic constants of this model to be

\[ C_{11} = \frac{a}{2r_0}, \]
\[ C_{12} = \frac{a}{2r_0} \left( \frac{2b}{a} - 1 \right), \] (9.4)
\[ C_{44} = \frac{a}{2r_0} \left( 1 - \frac{b^2}{a^2} \right), \]

which are independent of the size of crystal. At microscopic level, the apparent change of elastic moduli simply means that continuum mechanics is no longer able to fit the experimental results, and the fit, after the change of material constants, is no longer meaningful. Because it is beyond the region that the long-acoustic-wave-limit method applies, and the long-acoustic-wave-limit is where the continuum mechanics formulation comes from.

On the other hand, the micromachined devices based on a top–down approach fabrication, in contrast to most of the nano devices that are fabricated by bottom–up approaches, are well suited to the continuum treatment. Microcontinuum theory (micromorphic and micropolar) provides just the necessary and adequate tools and has advantages over either atomic model or classical continuum theories in such applications.

9.4.2. Piezoelectricity and ferroelectricity

The phenomenon of piezoelectricity is a consequence of electro-mechanical coupling. For a lattice to display the coupling, a necessary property is that the particle should carry an electrical charge. The displacement of particle possessing an electrical charge creates electrical dipoles. A summation and an averaging of the dipoles at the particle level leads to the macroscopic polarization field. So, the second essential property is that the crystal does not possess a center of
symmetry, such that the microscopic dipoles do not cancel each other out when averaged over a unit cell.

The displacement \( \mathbf{u}(l) \), \( \mathbf{u}(l') = \mathbf{u}(l) + \mathbf{u}(l\alpha) \), of the lattice point at \( x(l) \) with an electrical charge \( Z_s \) induces the dipole

\[
\mathbf{p}(l, \alpha) = Z_s \mathbf{u}(l, \alpha),
\]

(9.5)

and the dipole density per volume is defined as the polarization field,

\[
P_i = \frac{1}{V} \sum \mathbf{Z}_s \mathbf{u}_i(l, \alpha),
\]

(9.6)

where \( \mathbf{u}(l) \) is the displacement of \( \alpha \)th particle in the \( l \)th unit cell, \( \mathbf{u}(l) \) is the displacement of the center of \( l \)th unit cell, \( \mathbf{u}(l\alpha) \) is the displacement of \( \alpha \)th particle relative to the center of the \( l \)th unit cell.

The Coulomb interaction between the particles at the positions \( x(l, \alpha) \) and \( x(l', \alpha') \) with the electrical charges \( Z_s \) and \( Z_{s'} \), respectively, is

\[
\nu^C = \frac{Z_s Z_{s'}}{4\pi} \frac{1}{\left| x(l, \alpha) - x(l', \alpha') \right|}.
\]

(9.7)

The resultant force is mainly of an attractive type balanced by a repulsion force of short range. The second type of force is of quantum mechanical origin and is basically due to the repulsion of the electron clouds around its nearest neighbors. A semiempirical expression for the repulsive part of the interaction is provided by the Born potential:

\[
\nu^B = B \exp \left[ -\mu \left| x(l, \alpha) - x(l', \alpha') \right| \right].
\]

(9.8)

The total interaction potential for the lattice becomes

\[
V = \nu^C + \nu^B.
\]

(9.9)

The kinetic energy is given in the form

\[
T = \frac{1}{2} \sum_{l\alpha} m_s \mathbf{\dot{u}}_i(l, \alpha) \mathbf{\dot{u}}_i(l, \alpha).
\]

(9.10)

The dynamical equations are obtained from the Lagrangian \( L = T - V \) with \( T \) and \( V \) given above and can be expressed in the form [3]
\[ m_i \ddot{u}_i(l, x) = \sum_{l' \neq l} \phi_{ij} \left( l, l'; x, x' \right) u_j(l', x') + Z_i E_i(l, x). \]  

(9.11)

where \( \phi_{ij} \) is the internal force constant as a summation of the short range coefficient and the analytical part of the Coulomb interaction, and \( E_i(l, x) \) is the electrical field.

Clearly, from the microscopic viewpoint there is only one kind kinetic variable: the displacements of the lattice particle, \( u(l, x) \), which can be decomposed as \( u(l) \), the displacement of the center (macromotion), and \( u(l, x) \), the relative displacement of \( x \)th particle relative to the center (micromotion).

The above equations are to be complemented by the macroscopic Maxwell equations

\[ \nabla \cdot E = -4\pi \nabla \cdot P \]  

(9.12)

For plane wave solution of the form \( (E, P) = (E, P) \exp[i(q \cdot x_{tot})] \), the Maxwell equations yield

\[ E_i(l) = -4\pi \frac{q_i q_j}{|q|^2} P_j(l). \]  

(9.13)

The macroscopic piezoelectricity theory is the continuum long wave limit of the acoustic branch where the identity of the particles disappears by

\[ \lim_{q \to 0} u \left( l, x \right) \to u(l). \]

The displacements within the unit cell, which has created the dipole, are thus ignored. Further, the long wave limit method could not give \( E \) as an analytical function of \( P \) since

\[ \lim_{q_1, q_3 \to 0} \frac{q_1^2}{(q_1^2 + q_2^2 + q_3^2)} = 1, \]  

(9.14)

while

\[ \lim_{q_1, q_3 \to 0} \frac{q_1^2}{(q_1^2 + q_2^2 + q_3^2)} = 0. \]  

(9.15)

Further assumptions are thus needed. Apparently the long wave limit method would break down for a crystal with a small number of unit cells, and in small length scale the material moduli will no longer be constant, in fact they vary with the displacement or strain. Hence the nonlinearity will be observed. On the other hand, it is obvious that the continuum treatment by micromorphic theory takes the exact form of discrete lattice dynamics without the long acoustic wavelength assumption, and retains all the basic features presented in the discrete equations of lattice dynamics.

Also, for piezoelectricity, the only source of polarization is the displacement of the lattice point. Conversely, in ferroelectric crystals a permanent dipole exists in each cell. For example, in the
ferroelectrics of displacive type, such as BaTiO₃, one of the ions is shifted with respect to the center of symmetry of the unit cell. The result is a permanent dipole with magnitude equal to the shift distance multiplied by the charge of the ion. In these crystals the changes in the permanent dipole orientations result in a change in the polarization field. The polarization field of a permanent dipole, \( P_0 \), rotated by an angle \( \psi \) in the \( xy \)-plane about \( z \)-axis is

\[
P = \frac{P_0}{V_a} \begin{vmatrix} \cos \psi \\ \sin \psi \\ 0 \end{vmatrix}.
\]  

This is a motion within a unit cell, which results in at least a change of the orientation of the microstructure. Obviously, the continuum theories that ignore the microstructure are not suited for the description of this phenomenon. Even, for a macroscopic problem, the treatment of this rotation by a macroscopic continuum theory requires at least a nonlinear theory and more approximations will be encountered. On the other hand, displacive phase transition, as occurred in the ferroelectric crystals, is the results of the change of the microinertia tensor with temperature. The balance law of microinertia tensor distinguishes micromorphic theory from all other continuum theories. The change of polarization in ferroelectricity is a physical problem that can demonstrate the unique applicability of micromorphic theory.

Moreover, it can be seen that the link between lattice dynamics and micromorphic theory provides a chance to determine all the material constants in micromorphic piezoelectric and ferroelectric solids based on the information of above mentioned potential \( V^B \) and \( V^C \).

Those are the ongoing studies. Application of piezoelectricity and ferroelectricity will provide examples to show the power and practicality of micromorphic theory.

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