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An asymmetric theory of nonlocal elasticity—Part 1. Quasicontinuum theory

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Abstract

In this article, an asymmetric theory of nonlocal elasticity is developed on the basis of three dimensional atomic lattice model, the Galileo invariance for constitutive equations and by use of Fourier transformation of generalized function and energy method. It is shown that nonlocal characteristic functions (or constitutive parameters of internal elastic energy) can be explicitly expressed in terms of interacting forces connecting atoms, and the general model of nonlocal theory with rotation effects is asymmetric. Both symmetric stress and anti-symmetric stress is a nonlocal function of strain and local rotation for anisotropic materials. For isotropic materials, symmetric stress is only a nonlocal function of strain, while antisymmetric stress is only a nonlocal function of strain. All rights reserved.

1. Introduction

W. Voigt assumed that the transfer of interaction between two neighborhood elements of a body is not only by means of force vectors, but also by means of face moment vectors and body moment vectors; while the moment vectors make the stress tensor asymmetric (see Voigt, 1894). The displacement and rotation of a point in continuum media is correspondent with force and moment vectors respectively. Rotation in continuum mechanics can be divided into two kinds. One is independent rotation called micro-polar rotation. Another is anti-symmetric part of displacement gradient field called local rotation. Based on mechanical analysis between face moment acting on an infinitesimal element and the different rotation, the micro-polar theory and the couple stress theories have been developed respectively (see Cosserat, 1909; Mindlin and Tiersten, 1962; Eringen, 1976).

For asymmetric theories on the body moment (or body couple), Eringen (1976) first found out that the residual of nonlocal angular momentum, called the nonlocal body couple, can make stress asymmetric. But he ignored it. Kunin (1983) commenced on the theory of nonlocal symmetric quasi-continuum. "... a nonsymmetric stress tensor is necessarily associated with a weakly nonlocal theory of media of simple structure. This connected with the fact that in the above mentioned theories the stress tensor is introduced in a formal manner, by analogy with the local theory of

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elasticity and without due consideration of specific features of the nonlocal model". Gao and Tai (1990); Gao and Chen (1992) and Gao and Lin (1993) have derived the constitutive equation of nonlocal body moment associated with local rotation based on the axiom system of nonlocal continuum field and nonlocal quasicontinuum theory.

In this paper (which is Part 1 of nonlocal-asymmetric theory), the nonlocal asymmetric theory is studied based on atomic lattice model and the three dimensional quasicontinuum field theory, by use of Fourier transformation of generalized functions. First, the rotation effect on the internal energy of a body and integral form of the elastic internal energy from the restriction of the Galileo invariance for constitutive equations are examined. And then, the constitutive equation of asymmetric stress, divided into two parts: symmetric stress and antisymmetric stress, is derived, in which the constitutive parameters are dependent on micro-properties of atoms interconnecting. For anisotropic materials, both symmetric stress and antisymmetric stress are nonlocal functions of strain and local rotation. For isotropic materials, the symmetric stress is only a nonlocal function of strain, while the antisymmetric stress is only a nonlocal function of local rotation. In Part 2, we will develop the nonlocal-asymmetric theory based on the axiom system of nonlocal continuum field theory and investigate the relationship between nonlocal theory, higher gradient theory and couple stress theory.

2. The contribution of rotation to the internal energy of a body

In the atomic theory, covalent bonds existing in the interaction among the atoms are strongly oriented. A disturbance of lattice orientation at balance state excited by external moment makes the relative movements of neighboring atom lattices. The mechanical response of the relative movements can be represented by stretch springs and rotation springs, or by an elastic stick with both ends connecting to the neighboring atoms, as shown in Fig. 1 (see Jauhary, 1956).

Let us suppose a coordinate system in a three dimensional Euclidean space E_3 for the discrete lattice model with three covariant base vectors \mathbf{e}_{α} ($\alpha = 1,2,3$). The elementary volume constructed on \mathbf{e}_{α} forms a parallelepiped volume associated with an elementary cell of the lattice. Points of the lattice are called knots. The position vector of a lattice knot is expressed as $\mathbf{n} = n^{\alpha} \mathbf{e}_{\alpha}(n^{\alpha})$ is an arbitrary integer). The covariant metric tensor is equal to a scalar product of two covariant base vectors, i.e. $g_{\alpha\beta} = \mathbf{e}_{\alpha} \cdot \mathbf{e}_{\beta}$. The reciprocal to the covariant base vector \mathbf{e}_{α} is called the converse base vector, given by $\mathbf{e}_{\alpha} \cdot \mathbf{e}^{\beta} = \delta_{\alpha}^{\beta}$. The converse metric tensor is defined as $g^{\alpha\beta} = \mathbf{e}^{\alpha} \cdot \mathbf{e}^{\beta}$.

First the internal energy caused by atomic lattice rotations can be expressed as

$$\Phi_{\theta} = \Phi_{\theta}[\theta(\mathbf{n})] \tag{1}$$

here $\theta(\mathbf{n})$ (= $\theta^{\alpha} \mathbf{e}_{\alpha}$) is a rotation angle vector at the lattice knot \mathbf{n} .

For small rotation, Φ_{θ} can be expanded in a series of $\theta(\mathbf{n})$ as

$$\Phi_{\theta} = \psi_0 + \sum_{\mathbf{n}} \psi_1^{\lambda} \theta_{\lambda}(\mathbf{n}) + \frac{1}{2} \sum_{\mathbf{n}} \sum_{\mathbf{n}'} \psi_2^{\lambda \mu}(\mathbf{n}, \mathbf{n'}) \theta_{\lambda}(\mathbf{n}) \theta_{\mu}(\mathbf{n'}) + \dots$$
(2)

The constant ψ_0 , being the energy at a balance state can be ignored. In the neighborhood of balance position, $\psi_1^{\lambda}(\mathbf{n}) = 0$. Therefore, the first order approximation of the internal energy is



Fig. 1. (a) Rigid body rotation and (b) local rotation of deformable body (body couple m).

$$\Phi_{\theta} = \frac{1}{2} \sum_{\mathbf{n}} \sum_{\mathbf{n}'} \psi^{\lambda \mu}(\mathbf{n}, \mathbf{n'}) \theta_{\lambda}(\mathbf{n}) \theta_{\mu}(\mathbf{n'})$$
(3)

here the subscript 2 of $\psi_2^{\lambda\mu}(\mathbf{n},\mathbf{n'})$ is eliminated for convenience sake.

Due to the invariance of internal energy with respect to a rigid body rotation and the homogeneity assumption of a body, the parameters $\psi^{\lambda\mu}(\mathbf{n}, \mathbf{n'})$ have

(i)
$$\psi^{\lambda\mu}(\mathbf{n},\mathbf{n}') = \psi^{\lambda\mu}(|\mathbf{n}-\mathbf{n}'|)$$
 (4)

(ii)
$$\psi^{\lambda\mu}(0) = -\sum_{\mathbf{n}}' \psi^{\lambda\mu}(\mathbf{n}) \quad \text{or} \quad \sum_{\mathbf{n}} \psi^{\lambda\mu}(\mathbf{n}) = 0$$
 (5)

where Σ' indicates the summation, but $\mathbf{n} \neq \mathbf{0}$ (see Gao and Lin, 1992 for detailed discussion).

The consequent of eqn (4) and eqn (5) is

$$\sum_{\mathbf{n}}\sum_{\mathbf{n}'}\psi^{\lambda\mu}(\mathbf{n},\mathbf{n}')\theta_{\lambda}(\mathbf{n})\theta_{\mu}(\mathbf{n}) = \sum_{\mathbf{n}}\sum_{\mathbf{n}'}\psi^{\lambda\mu}(\mathbf{n},\mathbf{n}')\theta_{\lambda}(\mathbf{n}')\theta_{\mu}(\mathbf{n}') = 0$$
(6)

If we define that:

$$G^{\lambda\mu}(\mathbf{n}) = -\psi^{\lambda\mu}(\mathbf{n}); \quad \mathbf{n} \neq 0$$
(7)

The internal energy can be rewritten as

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$$\Phi_{\theta} = \frac{1}{4} \sum_{\mathbf{n}} \sum_{\mathbf{n}'} G^{\lambda \mu} (|\mathbf{n} - \mathbf{n'}|) [\theta_{\lambda}(\mathbf{n}) - \theta_{\mu}(\mathbf{n'})] [\theta_{\lambda}(\mathbf{n}) - \theta_{\mu}(\mathbf{n'})]$$
(8)

The internal energy associated with rotation(which can be either local rotation or polar rotation) can be expressed as a function of the difference of rotation angles of lattice knots representing relative rotation. The constitutive functions $G^{\lambda\mu}$ are determined by the gravitation feature among atoms and satisfy the binding condition given by eqn (5).

To develop a continuum model based on the behavior of atomic lattice model, we define the continuum field isomorphic to the discrete field, so that the value of continuum field at \mathbf{x} where the atom is located is equal to that of a discrete atom (or lattice knot). The continuum function can be obtained by the interpolating function in quasicontinuum field theory. The interpolating function is defined as

$$\delta_b(\mathbf{x}) = \frac{1}{(2\pi)^3} \int_B \exp(i\mathbf{x}.\mathbf{k}) \, \mathrm{d}\mathbf{k} = \frac{1}{\pi^3 V} \prod_{\beta=1}^3 \frac{\sin(\mathbf{x}_\beta \pi)}{\mathbf{x}_\beta} \tag{9}$$

where V_0 is the primitive cell's volume constructed by the frame $\{\mathbf{e}_{\alpha}\}$, B is parallelepiped, given by

$$B: [-\pi \leqslant \mathbf{k}_{\beta} \leqslant \pi; \beta = 1, 2, 3]$$

$$(10)$$

It is noted that the interpolating function $\delta_B(\mathbf{x})$ satisfies

$$\delta_B(0) = \frac{1}{V_0}; \quad \delta_B(\mathbf{n}) = 0 \quad (\mathbf{n} \neq \mathbf{0})$$
(11)

Any discrete function $f(\mathbf{n})$ converging rapidly with $|\mathbf{n}| \to \infty$ can be made to become a continuum function $f(\mathbf{x})$ by use of the above interpolating function $\delta_B(\mathbf{x})$ as follows

$$f(\mathbf{x}) = \sum_{\mathbf{n}} V_0 f(\mathbf{n}) \delta_B(\mathbf{x} - \mathbf{n})$$
(12)

The Fourier transform of the function $f(\mathbf{x})$ is given by

$$f(\mathbf{k}) = \int_{V_0} f(\mathbf{x}) \exp(-i\mathbf{k} \cdot \mathbf{x}) \, \mathrm{d}\mathbf{x}$$
(13)

According to the generalized function theory, the Fourier transform has established the simply isomorphic correspondence among topological spaces N(B) $(f(\mathbf{n}) \in N(B))$, X(B) $(f(\mathbf{x}) \in X(B))$ and K(B) $(f(\mathbf{k}) \in K(B))$. That is, the one-to-one correspondence $f(\mathbf{n}) \leftrightarrow f(\mathbf{x}) \leftrightarrow f(\mathbf{k})$ is well guaranteed by the condition of truncating the Fourier transform $f(\mathbf{k})$ of function $f(\mathbf{x})$ and the uniqueness of the expansion in eqn (12) and eqn (13). Due to properties of interpolating function $\delta_B(\mathbf{x})$, the continuum function $f(\mathbf{x}) has f(\mathbf{x})|_{\mathbf{x}=\mathbf{n}} = f(\mathbf{n})$. If the functions $g(\mathbf{n}) (\in N(B)), g(\mathbf{x}) (\in X(B))$ and $g(\mathbf{k}) (\in K(B))$, the Parseval equality gives the relation

$$\int_{V_0} \bar{f}(\mathbf{x}) g(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \int_B \bar{f}(\mathbf{k}) g(\mathbf{k}) \, \mathrm{d}\mathbf{k} = \sum_{\mathbf{n}} \bar{f}(\mathbf{n}) g(\mathbf{n}) \tag{14}$$

where $\bar{f}(\mathbf{x})$, $\bar{f}(\mathbf{k})$, $\bar{f}(\mathbf{n})$ are adjunct of complex functions $f(\mathbf{x})$, $f(\mathbf{k})$, $f(\mathbf{n})$.

According to the characteristics of the interaction among atoms, $G^{\lambda\mu}(|\mathbf{n}-\mathbf{n'}|)$ is a quick-decreasing function as the increase of $|\mathbf{n}-\mathbf{n'}|$. From the Parseval equality given by eqn (14), the internal energy associated with rotation can be expressed as the integral of continuous functions, given by

$$\Phi_{\theta} = \frac{1}{4} \int_{V} \int_{V} G^{\lambda \mu}(|\mathbf{x} - \mathbf{x}'|) \Theta_{\lambda}(\mathbf{x}, \mathbf{x}') \Theta_{\mu}(\mathbf{x}, \mathbf{x}') \, \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{x}'$$
(15)

where $\Theta_{\lambda}(\mathbf{x},\mathbf{x}') = \theta_{\lambda}(\mathbf{x}) - \theta_{\lambda}(\mathbf{x}')$; the continuous functions are given by

$$G^{\lambda\mu}(|\mathbf{x} - \mathbf{x}'|) = \sum_{\mathbf{n}} \sum_{\mathbf{n}'} V_0^2 G^{\lambda\mu}(|\mathbf{n} - \mathbf{n}'|) \delta_B(\mathbf{x} - \mathbf{n}) \delta_B(\mathbf{x}' - \mathbf{n}')$$

$$\theta_{\lambda}(\mathbf{x}) = \sum_{\mathbf{n}} V_0 \theta_{\lambda}(\mathbf{n}) \delta_B(\mathbf{x} - \mathbf{n})$$
(16)

The internal energy of rotation in continuum function space satisfies the Galileo invariance and has the same form as that obtained from asymmetric model of nonlocal continuum field theory (Gao and Tai, 1990). In addition, expanding the rotation $\theta_{\lambda}(\mathbf{x'})$ at \mathbf{x} leads to

$$\Phi_{\theta} = G^{\lambda\mu\alpha\beta} \partial_{\alpha} \theta_{\lambda}(\mathbf{x}) \partial_{\beta} \theta_{\mu}(\mathbf{x}) \tag{17}$$

which is the internal energy of rotation in the couple stress theory without couple terms of rotation with strain.

It has been shown that the location rotation makes a very important contribution to the internal energy and has different characteristics from rigid body rotation due to nonlocal effect. Also, the couple stress model can be regarded as the first order approximation of nonlocal theory with local rotation and specific model of higher gradient theory.

3. Elastic internal energy

According to the Born model of an atomic lattice regarded as a system of pointwise atomic particles situated at knots of the lattice, the elastic internal energy of the medium consisting of a group of atomic lattices is a function of displacement field $\mathbf{u}(\mathbf{n})$. For small displacement, the potential energy of the medium can be expressed as

$$\Phi = \frac{1}{2} \sum_{\mathbf{n}} \sum_{\mathbf{n}'} \Psi^{\lambda \mu}(\mathbf{n}, \mathbf{n}') u_{\lambda}(\mathbf{n}) u_{\mu}(\mathbf{n}')$$
(18)

where **u**(**n**) is the displacement of the atom at point **n**;

In eqn (18), $\Psi^{\lambda\mu}(\mathbf{n}, \mathbf{n}')$ are the constants constituting the parameters of the model called the force constants, connecting the atomic lattices at **n** and **n'**. And $\psi^{\lambda\mu}(\mathbf{n}, \mathbf{n}')$ has symmetry with respect to **n** and **n'**, i.e., $\Psi^{\lambda\mu}(\mathbf{n}, \mathbf{n}') = \Psi^{\mu\lambda}(\mathbf{n}', \mathbf{n})$. Due to the generalized function theory mentioned above, the internal energy can also be expressed as follows:

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$$\Phi = \frac{1}{2} \int_{V} \int_{V} \Psi^{\lambda\mu}(\mathbf{x}, \mathbf{x}') u_{\lambda}(\mathbf{x}) u_{\mu}(\mathbf{x}') \, d\mathbf{x} \, d\mathbf{x}'$$

$$= \frac{1}{(2\pi)^{3}} \int_{B} \int_{B} \Psi^{\lambda\mu}(\mathbf{k}, \mathbf{k}') u_{\lambda}(\mathbf{k}) u_{\mu}(\mathbf{k}') \, d\mathbf{k} \, d\mathbf{k}'$$
(19)

where

$$\Psi^{\lambda\mu}(\mathbf{k},\mathbf{k}') = \frac{1}{(2\pi)^3} \sum_{\mathbf{n}} \sum_{\mathbf{n}'} \Psi^{\lambda\mu}(\mathbf{n},\mathbf{n}') \exp(-(\mathbf{k}\cdot\mathbf{n}-\mathbf{k}'\cdot\mathbf{n}'))$$
$$= \frac{1}{(2\pi)^3} \int_{V} \int_{V} \Psi^{\lambda\mu}(\mathbf{x},\mathbf{x}') \exp(-(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{x}')) d\mathbf{x} d\mathbf{x}'$$
(20)

The internal energy should satisfy the Galileo invariance such that when a rigid body movement is superposed on a deformation body, its internal energy is invariable.

First, let us consider rectilinear uniform motion, given by

$$\mathbf{u}^*(\mathbf{x}) = \mathbf{u}(\mathbf{x}) + \mathbf{u}^0 \quad (\mathbf{u}^0 \text{ is a constant vector})$$
(21)

The Galileo invariance requires that

$$\Phi(\mathbf{u}) = \frac{1}{2} \int_{V} \int_{V} \Psi^{\lambda\mu}(\mathbf{x}, \mathbf{x}') u_{\lambda}(\mathbf{x}) u_{\mu}(\mathbf{x}') \, \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{x}'$$
$$= \frac{1}{2} \int_{V} \int_{V} \Psi^{\lambda\mu}(\mathbf{x}, \mathbf{x}') u_{\lambda}^{*}(\mathbf{x}) u_{\mu}^{*}(\mathbf{x}') \, \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{x}' = \Phi(\mathbf{u}^{*})$$
(22)

By substituting eqn (21) into eqn (22), expanding the two sides of the equation and eliminating the same terms, and then from the correlations among $\Psi^{\lambda\mu}(\mathbf{x}, \mathbf{x'})$, $\Psi^{\lambda\mu}(\mathbf{n}, \mathbf{n'})$ and $\Psi^{\lambda\mu}(\mathbf{k}, \mathbf{k'})$ and symmetry of $\Psi^{\lambda\mu}(\mathbf{k}, \mathbf{k'})$ with respect of \mathbf{k} and $\mathbf{k'}$, we can write $\Psi^{\lambda\mu}(\mathbf{k}, \mathbf{k'})$ as follows:

$$\Psi^{\lambda\mu}(\mathbf{k},\mathbf{k'}) = -k_{\alpha}k'_{\beta}c^{\lambda\mu\alpha\beta}(\mathbf{k},\mathbf{k'})$$

= $ik_{\alpha}ik'_{\beta}(c^{(\lambda\alpha)(\mu\beta)}(\mathbf{k},\mathbf{k'}) + c^{(\lambda\alpha)[\mu\beta]}(\mathbf{k},\mathbf{k'})) + ik_{\alpha}ik'_{\beta}(c^{[\lambda\alpha][\mu\beta]}(\mathbf{k},\mathbf{k'}) + c^{[\lambda\alpha](\mu\beta)}(\mathbf{k},\mathbf{k'}))$ (23)

By substituting eqn (23) into eqn (20) and from the properties of Parseval equation and Fourier transformation, the internal energy of quasicontinuum can be expressed as

$$\Phi = \frac{1}{2} \int_{V} \int_{V} \partial_{\lambda} u_{\alpha}(\mathbf{x}) \partial_{\mu'} u_{\beta}(\mathbf{x'}) [c^{(\lambda\alpha)(\mu\beta)}(\mathbf{x}, \mathbf{x'}) + c^{(\lambda\alpha)[\mu\beta]}(\mathbf{x}, \mathbf{x'}) + c^{[\lambda\alpha][\mu\beta]}(\mathbf{x}, \mathbf{x'}) + c^{[\lambda\alpha](\mu\beta)}(\mathbf{x}, \mathbf{x'})] d\mathbf{x} d\mathbf{x'} = \frac{1}{2} \int_{V} \int_{V} \partial_{(\lambda} u_{\alpha)}(\mathbf{x}) \partial_{(\mu'} u_{\beta)}(\mathbf{x'}) c^{(\lambda\alpha)(\mu\beta)}(\mathbf{x}, \mathbf{x'}) d\mathbf{x} d\mathbf{x'}$$

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$$+\frac{1}{2}\int_{V}\int_{V}\partial_{(\lambda}u_{\alpha)}(\mathbf{x})\partial_{(\mu}u_{\beta]}(\mathbf{x}')c^{(\lambda\alpha)[\mu\beta]}(\mathbf{x},\mathbf{x}')\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'$$

$$+\frac{1}{2}\int_{V}\int_{V}\partial_{[\lambda}u_{\alpha]}(\mathbf{x})\partial_{(\mu}u_{\beta)}(\mathbf{x}')c^{[\lambda\alpha](\mu\beta)}(\mathbf{x},\mathbf{x}')\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'$$

$$+\frac{1}{2}\int_{V}\int_{V}\partial_{(\lambda}u_{\alpha)}(\mathbf{x})\partial_{[\mu}u_{\beta]}(\mathbf{x}')c^{(\lambda\alpha)[\mu\beta]}(\mathbf{x},\mathbf{x}')\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'$$
(24)

where () indicates the symmetrization of indices, [] indicates the anti-symmetrization of indices. Then, let us consider a rigid body rotation superposed upon the body. We define

$$\mathbf{u}^*(\mathbf{x}) = \mathbf{u}(\mathbf{x}) + \boldsymbol{\omega}_0 \times \mathbf{x} \quad (\boldsymbol{\omega}_0 \text{ is a constant vector})$$
(25)

by substituting eqn (25) into eqn (24) and due to Galileo invariance, the constitutive functions $c^{(\lambda\alpha)[\mu\beta]}(\mathbf{x}, \mathbf{x'}), c^{[\lambda\alpha](\mu\beta)}(\mathbf{x}, \mathbf{x'})$ and $c^{[\lambda\alpha][\mu\beta]}(\mathbf{x}, \mathbf{x'})$ have to satisfy

$$\int_{V} c^{(\lambda \alpha)[\mu \beta]}(\mathbf{x}, \mathbf{x}') \, \mathrm{d}\mathbf{x}' = \mathbf{0}$$

$$\int_{V} c^{[\lambda \alpha][\mu \beta]}(\mathbf{x}, \mathbf{x}') \, \mathrm{d}\mathbf{x} = \mathbf{0}$$

$$\int_{V} c^{[\lambda \alpha][\mu \beta]}(\mathbf{x}, \mathbf{x}') \, \mathrm{d}\mathbf{x} = \mathbf{0}$$

$$\int_{V} c^{[\lambda \alpha][\mu \beta]}(\mathbf{x}, \mathbf{x}') \, \mathrm{d}\mathbf{x}' = \mathbf{0}$$
(26)

(See Gao and Lin (1993) for detailed discussion).

In this case, we can rewrite the internal energy of a quasicontinuum medium as follows

$$\Phi = \frac{1}{2} \int_{V} \int_{V} \partial_{(\lambda} u_{\alpha)}(\mathbf{x}) \partial_{\mu} u_{\beta)}(\mathbf{x}') c^{(\lambda \alpha)(\mu \beta)}(\mathbf{x}, \mathbf{x}') \, d\mathbf{x} \, d\mathbf{x}'$$

$$+ \frac{1}{2} \int_{V} \int_{V} \partial_{(\lambda} u_{\alpha)}(\mathbf{x}) (\theta_{\kappa}(\mathbf{x}') - \theta_{\kappa}(\mathbf{x})) C^{(\lambda \alpha)\kappa}(\mathbf{x}, \mathbf{x}') \, d\mathbf{x} \, d\mathbf{x}'$$

$$+ \frac{1}{2} \int_{V} \int_{V} \partial_{(\mu'} u_{\beta)}(\mathbf{x}') (\theta_{\kappa}(\mathbf{x}) - \theta_{\kappa}(\mathbf{x}')) C^{\kappa(\mu\beta)}(\mathbf{x}, \mathbf{x}') \, d\mathbf{x} \, d\mathbf{x}'$$

$$+ \frac{1}{4} \int_{V} \int_{V} (\theta_{\kappa}(\mathbf{x}) - \theta_{\kappa}(\mathbf{x}')) (\theta_{\iota}(\mathbf{x}') - \theta_{\iota}(\mathbf{x})) C^{\kappa\iota}(\mathbf{x}, \mathbf{x}') \, d\mathbf{x} \, d\mathbf{x}'$$
(27)

here

$$\theta_{\alpha} = \frac{1}{2} \epsilon_{\alpha}^{\beta\gamma} \partial_{[\beta} u_{\gamma]}$$

$$C^{\kappa(\mu\beta)} = \epsilon_{\lambda\alpha}^{\cdot\kappa} c^{[\lambda\alpha](\mu\beta)}$$

$$C^{(\lambda\alpha)\kappa} = \epsilon_{\mu\beta}^{\cdot\kappa} c^{(\lambda\alpha)[\mu\beta]}$$

$$C^{\kappa_{I}} = \epsilon_{\lambda\alpha}^{\cdot\kappa} \epsilon_{\mu\beta}^{\cdot\gamma} c^{[\lambda\alpha][\mu\beta]}$$
(28)

and $\in_{\alpha}^{\beta\gamma}$, $\in_{\alpha\beta}^{\gamma}$ are Eddington tensors.

The internal energy consists of three parts: strain energy, internal energy of local rotation and internal energy from coupling of strain and local rotation. If the coupling action of strain and local rotation is neglected, we have

$$\Phi = \frac{1}{2} \int_{V} \int_{V'} \partial_{(\lambda} u_{\alpha)}(\mathbf{x}) \partial_{(\mu} u_{\beta)}(\mathbf{x'}) c^{(\lambda \alpha)(\mu \beta)}(\mathbf{x}, \mathbf{x'}) \, \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{x'} + \frac{1}{4} \int_{V} \int_{V'} (\theta_{\kappa}(\mathbf{x}) - \theta_{\kappa}(\mathbf{x'})) (\theta_{i}(\mathbf{x'}) - \theta_{i}(\mathbf{x})) C^{\kappa i}(\mathbf{x}, \mathbf{x'}) \, \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{x'}$$
(29)

which is exactly the same as the potential energy obtained from the asymmetric theory of nonlocal elasticity (Gao and Tai, 1990).

In fact, for isotropic materials, the constitutive parameters $C^{(\lambda\alpha)\kappa}$, $C^{\kappa(\mu\beta)}$ should be isotropic tensors of third rank. From the representative theorem of isotropic tensors, the third rank isotropic tensor is $b \in \lambda^{\mu\kappa}$ (b is a constant) with the anti-symmetry of indices. Therefore, $C^{(\lambda\alpha)\kappa}$, $C^{\kappa(\mu\beta)}$ are equal to zero. Also eqn (29) can be regarded as internal energy of isotropic material. For anisotropic materials, the distortion effects between local rotation and symmetric stress, strain and antisymmetric stress play an important role in the internal energy. If the effect of local rotation is neglected, the potential energy is reduced to the classic model of nonlocal quasicontinuum field (Kunin, 1983).

4. Constitutive law and field equations

To derive the constitutive equations and field equations in the quasicontinuum field theory, we define the Lagrangian of the Born model system as follows

$$L = \frac{1}{2}g^{\alpha\beta}\sum_{\mathbf{n}}m(\mathbf{n})\dot{u}_{\alpha}(\mathbf{n})\dot{u}_{\beta}(\mathbf{n}) - \frac{1}{2}\sum_{\mathbf{n}}\sum_{\mathbf{n}'}\Psi^{\alpha\beta}(\mathbf{n},\mathbf{n'})u_{\alpha}(\mathbf{n})u_{\beta}(\mathbf{n'}) - \sum_{\mathbf{n}}q^{\alpha}(\mathbf{n})u_{\alpha}(\mathbf{n})$$
(30)

where $m(\mathbf{n})$ is the mass of the atom at point \mathbf{n} ; $q^{\alpha}(\mathbf{n})$ is the external force applied to the atom at point \mathbf{n} ; $\mathbf{\dot{u}}(\mathbf{n})$ is a velocity vector of the atom at point \mathbf{n} .

According to the Parseval equation, the Lagrangian L can be expressed as an integral of continuum functions as follows

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$$L = \frac{1}{2} \int_{V} \int_{V'} g^{\alpha\beta} \rho(\mathbf{x}) \dot{u}_{\alpha}(\mathbf{x}) \dot{u}_{\beta}(\mathbf{x}') \delta(\mathbf{x} - \mathbf{x}') \, \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{x}' - \frac{1}{2} \int_{V} \int_{V'} \Psi^{\alpha\beta}(\mathbf{x}, \mathbf{x}') u_{\alpha}(\mathbf{x}) u_{\beta}(\mathbf{x}') \, \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{x}' - \int_{V} q^{\alpha}(\mathbf{x}) u_{\alpha}(\mathbf{x}) \, \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{x}$$

$$- \int_{V} q^{\alpha}(\mathbf{x}) u_{\alpha}(\mathbf{x}) \, \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{x}$$
(31)

The motion equation is obtained by the energy principle that of all admissive movements, the real movement can be distinguished by the variational equation that $\delta L = 0$ and is given by

$$\rho(\mathbf{x})\ddot{u}^{\alpha}(\mathbf{x}) + \int_{V} \Psi^{\alpha\beta}(\mathbf{x}, \mathbf{x}') u_{\beta}(\mathbf{x}') \, \mathrm{d}\mathbf{x}' = q^{\alpha}(\mathbf{x})$$
(32)

From the Parseval equation and the Galileo invariance discussed in previous section, the Fourier transform of the second term in eqn (32), which is an integral defined as I, can be expressed as follows

$$F[I] = \frac{1}{(2\pi)^3} \int_B \Psi^{\alpha\beta}(\mathbf{k}, \mathbf{k'}) u_\beta(\mathbf{k'}) \, \mathrm{d}\mathbf{k'}$$
$$= \frac{1}{(2\pi)^3} \int_B i k_\lambda i k_\mu c^{\lambda\alpha\mu\beta}(\mathbf{k}, \mathbf{k'}) u_\beta(\mathbf{k'}) \, \mathrm{d}\mathbf{k'}$$
(33)

Due to formulae of Fourier transformation, the inverse transformation of F[I] gives

$$I = \partial_{\lambda} \int_{V} c^{\lambda \alpha \mu \beta}(\mathbf{x}, \mathbf{x'}) (\partial_{\mu} u_{\beta}(\mathbf{x'})) \, \mathrm{d}\mathbf{x'}$$
(34)

By substituting eqn (34) into the previous motion equation given by eqn (32), we obtain

$$\rho(\mathbf{x})\ddot{u}^{\alpha}(\mathbf{x}) + \partial_{\lambda}\sigma^{\lambda\alpha}(\mathbf{x}) = q^{\alpha}(\mathbf{x})$$
(35)

where the constitutive equation is

$$\sigma^{\lambda\alpha}(\mathbf{x}) = \int_{V} c^{\lambda\alpha\mu\beta}(\mathbf{x}, \mathbf{x}') (\partial_{\mu} u_{\beta}(\mathbf{x}')) \, \mathrm{d}\mathbf{x}'$$
(36)

It is noted that the motion equation is similar to that of classic elasticity; but the constitutive equation of stress is different and can be decomposed into two parts: symmetric and antisymmetric. In addition, from the restriction conditions on constitutive parameters $c^{(\lambda\alpha)[\mu\beta]}(\mathbf{x}, \mathbf{x}')$, $c^{[\lambda\alpha](\mu\beta)}(\mathbf{x}, \mathbf{x}')$ and $c^{[\lambda\alpha][\mu\beta]}(\mathbf{x}, \mathbf{x}')$ given by the Galileo invariance and the homogeneity, assumption of materials requires that $c^{\lambda\alpha\mu\beta}(\mathbf{x}, \mathbf{x}') = c^{\lambda\alpha\mu\beta}(|\mathbf{x} - \mathbf{x}'|)$ etc., both symmetric stress and antisymmetric stress can be expressed explicitly in terms of nonlocal functions of strain and local rotation given by

$$\sigma^{\lambda\alpha}(\mathbf{x}) = \sigma^{(\lambda\alpha)}(\mathbf{x}) + \sigma^{[\lambda\alpha]}(\mathbf{x})$$
(37)

and

$$\sigma^{(\lambda\alpha)}(\mathbf{x}) = \int_{V} c^{(\lambda\alpha)(\mu\beta)}(|\mathbf{x}-\mathbf{x'}|)\partial_{(\mu}u_{\beta)}(\mathbf{x'})\,\mathrm{d}\mathbf{x'} + \int_{V} C^{(\lambda\alpha)\delta}(|\mathbf{x}-\mathbf{x'}|)(\theta_{\delta}(\mathbf{x'})-\theta_{\delta}(\mathbf{x}))\,\mathrm{d}\mathbf{x'}$$

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$$\sigma^{[\lambda\alpha]}(\mathbf{x}) = \int_{V} c^{[\lambda\alpha](\mu\beta)}(|\mathbf{x} - \mathbf{x}'|)\partial_{(\mu}u_{\beta)}(\mathbf{x}')\,\mathrm{d}\mathbf{x}' + \int_{V} C^{[\lambda\alpha]\delta}(|\mathbf{x} - \mathbf{x}'|)(\theta_{\delta}(\mathbf{x}') - \theta_{\delta}(\mathbf{x}))\,\mathrm{d}\mathbf{x}'$$
(38)

where

$$C^{[\lambda\alpha]\delta}(|\mathbf{x} - \mathbf{x}'|) = \epsilon^{\sigma\delta}_{\mu\beta} c^{[\lambda\alpha][\mu\beta]}(|\mathbf{x} - \mathbf{x}'|)$$

$$C^{(\lambda\alpha)\delta}(|\mathbf{x} - \mathbf{x}'|) = \epsilon^{\sigma\delta}_{\mu\beta} c^{(\lambda\alpha)[\mu\beta]}(|\mathbf{x} - \mathbf{x}'|)$$
(39)

For isotropic materials, the constitutive parameters $c^{\lambda\alpha\mu\beta}$ and $C^{\lambda\alpha\mu}$ are isotropic tensors. So, the constitutive equations of symmetric stress and antisymmetric stress can be expressed as follows:

$$\sigma^{(\iota\alpha)}(\mathbf{x}) = \int_{V} (c_1(|\mathbf{x} - \mathbf{x}'|)g^{\lambda\alpha}\partial_{(\beta}u_{\beta)}(\mathbf{x}') + [c_2(|\mathbf{x} - \mathbf{x}'|) + c_3(|\mathbf{x} - \mathbf{x}'|)]g^{\lambda\mu}g^{\alpha\beta}\partial_{(\beta}u_{\mu)}(\mathbf{x}'))\iota$$

$$\sigma^{[\lambda\alpha]}(\mathbf{x}) = \epsilon^{\lambda\alpha\delta} \int_{V} C_0(|\mathbf{x} - \mathbf{x}'|)(\theta_{\delta}(\mathbf{x}') - \theta_{\delta}(\mathbf{x}))\,\mathrm{d}\mathbf{x}'$$
(40)

The constitutive equation of symmetric stress has the same form as that proposed by Eringen (1976). As discussed in section 3, the constitutive parameters $c_i(|\mathbf{x} - \mathbf{x'}|)(i = 1,2,3)$ and $C_0(|\mathbf{x} - \mathbf{x'}|)$ called as the nonlocal characteristic functions are determined by the gravitation feature among interacting atoms, i.e. they decrease rapidly as the increase of $|\mathbf{x} - \mathbf{x'}|$. For example, from the quasicontinuum theory (see Kunin 1983), the one dimensional nonlocal characteristic function $C_0(|\mathbf{x}|)$ can be expressed as follows

$$C_0(x) = \sum_{\mathbf{n}} C(n)\delta_B(x - na)$$
(41)

where C(n) is interacting moment connecting atomic lattices at points n and 0. And

$$\delta_B(x) = \frac{\sin\left(\frac{x}{\pi}\right)}{\pi x}; \quad |x| \le a$$

$$= 0; \quad |x| \ge a$$
(42)

If the interaction of the nearest atom is only considered, $C_0(|x|)$ is explicitly expressed as follows

$$C_0(x) = C_0 \delta_B(x) = C_0 \frac{\sin\left(\frac{\pi}{a}x\right)}{\pi x}; \quad |x| \le a$$

= 0; $|x| \ge a$ (43)

A linear approximation of the nonlocal characteristic function $C_0(|x|)$ can be made by the linear function given by



$$C_0(x)\frac{a}{C_0} = 1 - \frac{|x|}{a}; \quad |x| \le a$$

$$= 0; \quad |x| \ge a$$
(44)

Figure 2 shows that both characteristic functions of $C_0(|x|)$ have a gravitation feature. A more detailed discussion on it can be found in the previous work (Gao and Chen, 1992).

It is noted that the due physical variable of the rotation is moment. Therefore, the nonlocal moment can be defined as nonlocal function of local rotation, given by

$$\rho L_{\delta}(\mathbf{x}) = \int_{V} C_0(|\mathbf{x} - \mathbf{x}'|)(\theta_{\delta}(\mathbf{x}') - \theta_{\delta}(\mathbf{x})) \, \mathrm{d}\mathbf{x}'$$
(45)

the antisymmetric stress has the relationship with the moment vector, given by

$$\rho L_{\delta}(\mathbf{x}) = \frac{1}{2} \epsilon_{\lambda \alpha \delta} \sigma^{[\lambda \alpha]}(\mathbf{x}) \tag{46}$$

In fact, the moment is residual of nonlocal moment of angular momentum in continuum field theory of nonlocal elasticity, which is nonlocal function of local rotation. For the rigid body rotation, $\rho L_{\delta}(\mathbf{x}) = 0$.

5. Discussion

In this paper, the asymmetric theory of nonlocal elasticity has been developed on the basis of quasicontinuum theory. The asymmetric stress can be decomposed into symmetric stress and antisymmetric stress. Both symmetric stress and anti-symmetric stress for anisotropic materials are nonlocal functions of strain and difference of local rotation for anisotropic materials. For isotropic material, the symmetric stress is a function of strain and anti-symmetric stress is a nonlocal function of local relative rotation. The nonlocal constitutive functions, such as $c^{(\lambda \alpha)[\mu\beta]}(|\mathbf{x} - \mathbf{x}'|)$,

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 $c^{(\lambda\alpha)(\mu\beta)}(|\mathbf{x}-\mathbf{x'}|), c^{[\lambda\alpha][\mu\beta]}(|\mathbf{x}-\mathbf{x'}|)$ and $c^{[\lambda\alpha](\mu\beta)}(|\mathbf{x}-\mathbf{'}|)$ etc., are dependent of micro- behavior of atoms lattice. It is verified that the nonlocal body moment exists, plays a very important role in a deformed body. It is also shown that both strain and local rotation should be regarded as basic variables of geometric deformation. The correspondence deformation mechanism between stresses and local rotation is nonlocal and dependent of micro-behaviors of inter-atoms.

In the zone of localized deformation, such as a kink band and a shear band, the local rotation is significantly large, the material is not isotropic, and the orientation of a lattice is very sensitive to an external load. The developed asymmetric model of nonlocal theory provides a useful method for studying the localized deformation phenomena because the model can describe the influence of orientation of a lattice on the stress status.

It is noted that the asymmetric theory of nonlocal elasticity is a more general model, which is based on the general case that both strain and local rotation are considered without any simplifying assumptions. If the effect of local rotation is neglected, the model can be reduced to Kroner-Eringen model in nonlocal elasticity. If the nonlocal effect is neglected, the anti-symmetric stress is also zero and constitutive equation of symmetric stress degenerates into that in classic elasticity. Further discussion of nonlocal-asymmetric theory will be shown in Part 2.

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