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Derivation of macroscopic relations of the elasticity of complex crystal lattices taking into account the moment interactions at the microlevel☆

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Abstract

A discrete mechanical model of a complex crystal lattice is proposed which contains particles possessing both translational and rotational degrees of freedom and which interact with one another by means of forces and moments. The transition to a continuum model of a crystal lattice is performed using the long-wave approximation, and, at the same time, it is shown that the dynamics of the continual model are described by the equations of the macroscopic moment theory of elasticity. Expressions are obtained for the macroscopic stiffness tensors which depend on the stiffness tensors of the interatomic bonds and the vectors determining the lattice geometry. A transition to the moment less theory of elasticity is made and it is shown that the macroscopic moduli of elasticity of the moment less theory depend both on the forces and the torque characteristics of the interatomic interaction. The stiffnesses of the interatomic bonds in a layer of graphite are calculated and it is shown that the transverse stiffness of an interatomic bond is comparable with the longitudinal stiffness, that is, a covalent bond is substantially non- central, which is only possible when there are torque interactions at the microlevel.

Paired interaction potentials such as the Lennard-Jones, Mie and Morse potentials, are extensively used when solving problems in continuums mechanics by the methods of molecular dynamics. These potentials have a clear physical meaning and enable one to describe the thermomechanical properties of many materials at a qualitative level. However, it is well known that paired potentials, as a rule, can only ensure the stability of closely packed crystal lattices. Lattices with a lower packing density are found to be unstable for the majority of paired potentials. For example, structures which are characteristic of covalent crystals such as an hexagonal lattice in a plane (the structure of graphite) and the spatial structure of diamond are unstable. The traditional solution to this problem consists of using multiparticle interaction potentials[1,2] that depend on the angles between bonds, which enables one to make structures with a low filling density stable. However, the form of such potentials turns out to be very complex and the physical meaning of the parameters occurring in them is unclear.

An alternative approach consists of introducing rotational degrees of freedom into the treatment and taking account of the torque contribution in the interatomic interaction.[3,4] Taking the example of simple crystal lattices, it has been shown[3,4] that by taking account of the pairwise torque interaction (in addition to the pairwise force interaction) one

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can ensure the stability of crystal structures with a low packing density. A second approach has been developed in Refs 5,6 which is also associated with taking account of the rotational degrees of freedom. Below, the ideas in Refs 3,4 are extended to complex crystal lattices.* A method of describing the crystalline packing of the particles of a complex lattice is developed which enables one to obtain the linear moment theory of elasticity in the long-wave approximation.[7] At the same time, the approach in Refs 8–10 for the momentless case is used. In describing the moment interaction between particles, the greatest difficulty is in the introduction of measures of strain and in obtaining the constitutive equations.

The approach developed by Zhilin to construct moment theories in continuum mechanics[11–14] is used below to determine strain vectors and to obtain the constitutive equations for the interaction of the particles.

1. Description of interatomic interactions on the basis of moment theory

We shall model the atoms of a crystal lattice with particles which are point bodies. By a point body we mean[15] a material object of zero volume, the position of which is assumed to be defined if the position vector $\mathbf{R}(t)$ and the rotation tensor $\mathbf{P}(t)$ are given. The interaction between point bodies is characterized by a force vector and a torque vector. The dynamic structures and inertial characteristics of a point body are introduced in the following manner. The quadratic form of its translational and angular velocities $\mathbf{v}$ and $\boldsymbol{\omega}$

$$K = \frac{1}{2}m\mathbf{v}\cdot\mathbf{v} + \mathbf{v}\cdot\boldsymbol{\vartheta}\cdot\boldsymbol{\omega} + \frac{1}{2}\boldsymbol{\omega}\cdot\boldsymbol{\theta}\cdot\boldsymbol{\omega} \tag{1.1}$$

is called the kinetic energy of the point body. The second rank tensors ϑ and $\boldsymbol{\theta}$ are called the inertial tensors of the point body and m is the mass of the point body. The linear form of the velocities

$$\mathbf{K}_1 = \frac{\partial K}{\partial \mathbf{v}} = m\mathbf{v} + \boldsymbol{\vartheta}\cdot\boldsymbol{\omega} \tag{1.2}$$

is called the momentum of the point body.

The linear form

$$\mathbf{K}_2 = \frac{\partial K}{\partial \boldsymbol{\omega}} = \mathbf{v}\cdot\boldsymbol{\vartheta} + \boldsymbol{\theta}\cdot\boldsymbol{\omega} \tag{1.3}$$

is called the intrinsic angular momentum of the point body.

The quantity

$$\mathbf{K}_2^Q = (\mathbf{R} - \mathbf{R}_Q)\times\frac{\partial K}{\partial \mathbf{v}} + \frac{\partial K}{\partial \boldsymbol{\omega}} \tag{1.4}$$

is called the angular momentum of the point body calculated with respect to a reference point Q. We shall consider point bodies for which $\vartheta \equiv 0$ when modelling a crystal lattice below. For simplicity, we shall refer to them simply as particles.

Thus, we consider two interacting particles (Fig. 1) which simulate the atoms of a crystal lattice and determine the dependence of the force and the moment of the interaction of the particles on their mutual spacing and orientation, observing a complete analogy with what is done in the theory of shells and rods.[11,13]

In an actual configuration, the position of the particles is specified by the radius vectors $\mathbf{r}_1$ and $\mathbf{r}_2$, and the orientation is specified by the rotation vectors $\boldsymbol{\varphi}_1$ and $\boldsymbol{\varphi}_2$. In the equilibrium position,

$$\mathbf{r}_2 - \mathbf{r}_1 = \mathbf{r}_0, \quad \boldsymbol{\varphi}_1 = 0, \quad \boldsymbol{\varphi}_2 = 0$$

We now introduce the following notation: $\mathbf{F}_1$ and $\mathbf{M}_2$ are force and moment acting on particle 1 on the part of particle 2, $\mathbf{F}_2$ and $\mathbf{M}_2$ are the force and the moment acting on particle 2 on the part of particle 1, and $\mathbf{F}_1^e$, $\mathbf{M}_1^e$ and $\mathbf{F}_2^e$, $\mathbf{M}_2^e$ are the

* A crystal lattice in which all the nodes are equivalent is said to be simple (a simple cubic lattice). In other words, in the case of a simple lattice a displacement along a vector joining any two lattice points is an identity transformation. A lattice which does not possess this property is said to be complex (the graphite and diamond lattices, for example).[7]

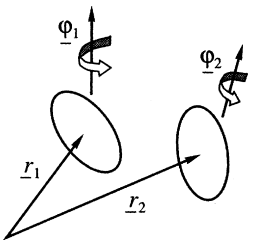

Fig. 1.

external actions on particles 1 and 2 respectively. The moments $\mathbf{M}_1$ and $\mathbf{M}_1^e$ are calculated with reference to particle 1, and the moments $\mathbf{M}_2$ and $\mathbf{M}_2^e$ are calculated with respect to particle 2.

We now write the equations of motion for particle 1, particle 2 and the system consisting of the two particles

$$\begin{aligned} &m_1\dot{\mathbf{v}}_1 = \mathbf{F}_1 + \mathbf{F}_1^e, \quad (\boldsymbol{\theta}_1 \cdot \boldsymbol{\omega}_1)^{\cdot} = \mathbf{M}_1 + \mathbf{M}_1^e, \quad m_2\dot{\mathbf{v}}_2 = \mathbf{F}_2 + \mathbf{F}_2^e, \quad (\boldsymbol{\theta}_2 \cdot \boldsymbol{\omega}_2)^{\cdot} = \mathbf{M}_2 + \mathbf{M}_2^e \\ &(m_1\mathbf{v}_1 + m_2\mathbf{v}_2)^{\cdot} = \mathbf{F}_1^e + \mathbf{F}_2^e \\ &(\mathbf{r}_1 \times m_1\mathbf{v}_1 + \boldsymbol{\theta}_1\boldsymbol{\omega}_1 + \mathbf{r}_2 \times m_2\mathbf{v}_2 + \boldsymbol{\theta}_2\boldsymbol{\omega}_2)^{\cdot} = \mathbf{r}_1 \times \mathbf{F}_1^e + \mathbf{M}_1^e + \mathbf{r}_2 \times \mathbf{F}_2^e + \mathbf{M}_2^e \end{aligned} \tag{1.5}$$

Here m_1, m_2 and $\boldsymbol{\theta}_1$, $\boldsymbol{\theta}_2$ are the masses and inertia tensors of the particles and $\mathbf{v}_1$, $\mathbf{v}_2$ and $\boldsymbol{\omega}_1$, $\boldsymbol{\omega}_2$ are their linear and angular velocities. Newton's third law for forces and the analogue of Newton's third law for moments are a corollary of Eq. (1.5):

$$\mathbf{F}_1 + \mathbf{F}_2 = 0, \quad \mathbf{r}_1 \times \mathbf{F}_1 + \mathbf{M}_1 + \mathbf{r}_2 \times \mathbf{F}_2 + \mathbf{M}_2 = 0 \tag{1.6}$$

We now note the energy balance equation for a system consisting of two particles

$$\begin{aligned} &\left(\frac{1}{2}[m_1\mathbf{v}_1 \cdot \mathbf{v}_1 + \boldsymbol{\omega}_1 \cdot \boldsymbol{\theta}_1 \cdot \boldsymbol{\omega}_1 + m_2\mathbf{v}_2 \cdot \mathbf{v}_2 + \boldsymbol{\omega}_2 \cdot \boldsymbol{\theta}_2 \cdot \boldsymbol{\omega}_2] + U\right)^{\cdot} = \\ &= \mathbf{F}_1^e \cdot \mathbf{v}_1 + \mathbf{M}_1^e \cdot \boldsymbol{\omega}_1 + \mathbf{F}_2^e \cdot \mathbf{v}_2 + \mathbf{M}_2^e \cdot \boldsymbol{\omega}_2 \end{aligned} \tag{1.7}$$

where U is the internal energy of the system (the interaction energy of particles 1 and 2). Assuming the displacements from the equilibrium position to be small quantities and taking account of Eqs. (1.5) and (1.6), the energy balance Eq. (1.7) can be reduced to the form

$$\begin{aligned} &\dot{U} = \mathbf{F} \cdot \dot{\boldsymbol{\varepsilon}} + \mathbf{M} \cdot \dot{\boldsymbol{\kappa}} \\ &\mathbf{F} = \mathbf{F}_1 = -\mathbf{F}_2, \quad \mathbf{M} = \mathbf{M}_1 + \frac{1}{2}(\mathbf{r}_1 - \mathbf{r}_2) \times \mathbf{F}_1 = -\mathbf{M}_2 - \frac{1}{2}(\mathbf{r}_2 - \mathbf{r}_1) \times \mathbf{F}_2 \\ &\boldsymbol{\varepsilon} = \mathbf{r} - \mathbf{r}_0 + \frac{1}{2}\mathbf{r}_0 \times (\boldsymbol{\varphi}_1 + \boldsymbol{\varphi}_2), \quad \boldsymbol{\kappa} = \boldsymbol{\varphi}_2 - \boldsymbol{\varphi}_1, \quad \mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1 \end{aligned} \tag{1.8}$$

Here $\mathbf{M}$ has the meaning of the moment acting on particle 1 on the part of particle 2, calculated with respect to the middle of the segment joining these particles. We shall call the vectors $\boldsymbol{\varepsilon}$ and $\boldsymbol{\kappa}$ in which the force vector and the moment vector perform work (see formulae (1.8)) strain vectors.

We next consider the elastic deformation of the system. We shall assume that the internal energy, the force vector and the moment vector depend solely on the strain vectors and are independent of the velocities. Then,

$$\mathbf{F} = \frac{\partial U}{\partial \boldsymbol{\varepsilon}}, \quad \mathbf{M} = \frac{\partial U}{\partial \boldsymbol{\kappa}} \tag{1.9}$$

Since the deformations are assumed to be small, the following approximation can be taken for the internal energy

$$U = \mathbf{F}^0 \cdot \boldsymbol{\varepsilon} + \mathbf{M}^0 \cdot \boldsymbol{\kappa} + \frac{1}{2}\boldsymbol{\varepsilon} \cdot \mathbf{A} \cdot \boldsymbol{\varepsilon} + \boldsymbol{\varepsilon} \cdot \mathbf{B} \cdot \boldsymbol{\kappa} + \frac{1}{2}\boldsymbol{\kappa} \cdot \mathbf{C} \cdot \boldsymbol{\kappa} \tag{1.10}$$

The coefficients **A**, **B** and **C** are called stiffness tensors, and $\mathbf{F}^0$ and $\mathbf{M}^0$ are the initial forces. In linear theory, stiffness tensors are constant quantities, and the tensors **A** and **C** are symmetric tensors, while the tensor **B** is an arbitrary tensor. According to formulae (1.9) and (1.10), the force vector and the moment vector have the form

$$\mathbf{F} = \mathbf{F}^0 + \mathbf{A}\cdot\boldsymbol{\varepsilon} + \mathbf{B}\cdot\boldsymbol{\kappa}, \quad \mathbf{M} = \mathbf{M}^0 + \boldsymbol{\varepsilon}\cdot\mathbf{B} + \mathbf{C}\cdot\boldsymbol{\kappa} \tag{1.11}$$

Starting from the theory of the symmetry of tensor quantities,[11] it can be shown that, if the internal structure of the particles is such that the system in the reference configuration is symmetric about two mutually perpendicular planes, the tensor **B** vanishes. This symmetry holds for the majority of the simplest crystal lattices.

The interaction moment **M**, calculated with reference to the middle of the segment joining the interacting particles, was used above in order to obtain elastic relations. At the same time, the stiffness tensors **B** and **C** also have the meaning of tensors calculated with reference to the middle of the segment joining the particles. This approach is convenient from the point of view of the application of symmetry theory to determine of the structure of the stiffness tensors. However, in deriving the equations of motion of a discrete medium, it is more convenient to use the interaction moments calculated with reference to the particles. Arguments, similar to those presented above, enable one to obtain the following description of the interaction of the particles using the interaction moment $\mathbf{M}_1$, which characterizes the action of particle 2 on particle 1 and is calculated with respect to particle 1

$$\begin{aligned} &\mathbf{F}_1 = \tilde{\mathbf{F}}^0 + \tilde{\mathbf{A}}\cdot\boldsymbol{\varepsilon}_1 + \tilde{\mathbf{B}}\cdot\boldsymbol{\kappa}_1, \quad \mathbf{M}_1 = \tilde{\mathbf{M}}^0 + \boldsymbol{\varepsilon}_1\cdot\tilde{\mathbf{B}} + \tilde{\mathbf{C}}\cdot\boldsymbol{\kappa}_1 \\ &\boldsymbol{\varepsilon}_1 = \mathbf{r} - \mathbf{r}_0 + \mathbf{r}_0\times\boldsymbol{\varphi}_2, \quad \boldsymbol{\kappa}_1 = \boldsymbol{\varphi}_2 - \boldsymbol{\varphi}_1, \quad \mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1 \end{aligned} \tag{1.12}$$

The stiffness tensors $\tilde{\mathbf{A}}$, $\tilde{\mathbf{B}}$, $\tilde{\mathbf{C}}$ and the initial forces $\tilde{\mathbf{F}}^0$ and $\tilde{\mathbf{M}}^0$ differ from the stiffness tensors **A, B** and **C** and the initial forces $\mathbf{F}^0$ and $\mathbf{M}^0$. It is easily shown that these quantities are connected with one another by the relations

$$\begin{aligned} &\tilde{\mathbf{F}}^0 = \mathbf{F}^0, \quad \tilde{\mathbf{M}}^0 = \mathbf{M}^0 + \frac{1}{2}\mathbf{r}_0\times\mathbf{F}^0 \\ &\tilde{\mathbf{A}} = \mathbf{A}, \quad \tilde{\mathbf{B}} = \mathbf{B} - \frac{1}{2}\mathbf{A}\times\mathbf{r}_0, \quad \tilde{\mathbf{C}} = \mathbf{C} + \frac{1}{2}(\mathbf{r}_0\times\mathbf{B} - \mathbf{B}^T\times\mathbf{r}_0) - \frac{1}{4}\mathbf{r}_0\times\mathbf{A}\times\mathbf{r}_0 \end{aligned} \tag{1.13}$$

2. The geometry of a crystal lattice

We will now consider a complex crystal lattice (Fig. 2). Particles, interacting by means of forces and moments (see formula (1.12)), form the lattice. It is assumed that each particle interacts with a limited number of neighbours. In the crystal, we pick out the Bravais lattice which decomposes the space into unit cells and consider a certain unit cell

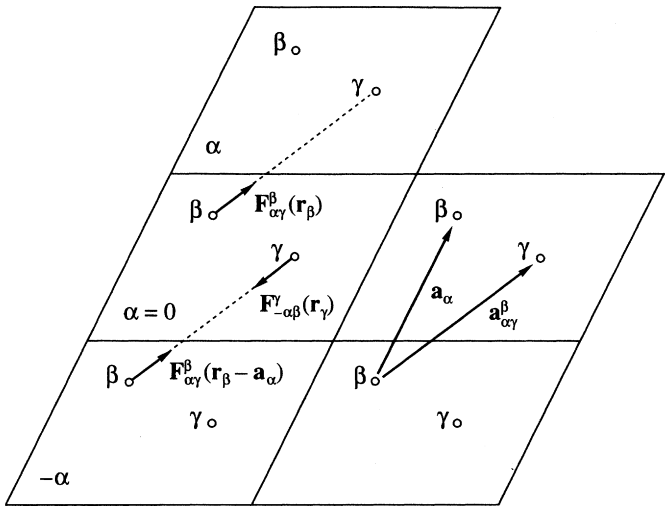

Fig. 2.

which, for convenience, we shall call the initial cell. We shall number all the cells in which there are atoms which interact with the atoms of the initial cell. We assign the number $\alpha = 0$ to the initial cell and the numbers $\alpha \pm 1, \pm 2, \ldots \pm N$ to the remaining cells. At the same time, the numbering is carried out in such a way that cells which are arranged symmetrically with respect to the initial cell have indices which are opposite in sign. We shall number the particles which occur in each cell with indices from 1 to M, where M is the number of particles in a unit cell. We will denote the radius vector defining the position of a particle γ in cell α with reference to a particle β of the initial cell in the reference configuration by $\mathbf{a}^{\beta}_{\alpha\gamma}$. The notation $\mathbf{a}_{\alpha} \equiv \mathbf{a}^{\beta}_{\alpha\beta}$ is used for brevity. It is easy to show that the property $\mathbf{a}^{\gamma}_{-\alpha\beta} = -\mathbf{a}^{\beta}_{\alpha\gamma}$ holds.

3. The equations of lattice particle dynamics

Assuming the displacements and rotations to be small quantities, we will write Euler's dynamical equations for a particle γ of the initial cell

$$m_{\gamma}\ddot{\mathbf{u}}_{\gamma} = \sum_{\alpha,\beta}\mathbf{F}^{\gamma}_{\alpha\beta} + \mathbf{f}^{*}_{\gamma}, \quad \boldsymbol{\theta}_{\gamma}\cdot\ddot{\boldsymbol{\varphi}}_{\gamma} = \sum_{\alpha,\beta}\mathbf{M}^{\gamma}_{\alpha\beta} + \mathbf{m}^{*}_{\gamma} \tag{3.1}$$

Here $\mathbf{u}_{\gamma}$ and $\boldsymbol{\varphi}_{\gamma}$ are the displacement vector and the rotation vector of the particle, m_{γ} and $\boldsymbol{\theta}_{\gamma}$ are the mass and inertial tensor, $\mathbf{F}^{\gamma}_{\alpha\beta}$ and $\mathbf{M}^{\gamma}_{\alpha\beta}$ are the force and the moment acting on particle γ of the initial cell due to particle β of cell α (Fig. 2) and the vectors $\mathbf{f}^{*}_{\gamma}$ and $\mathbf{m}^{*}_{\gamma}$ are the external actions. The moments $\mathbf{M}^{\gamma}_{\alpha\beta}$ and $\mathbf{m}^{*}_{\gamma}$ were calculated with reference to particle γ of the initial cell. The equations

$$\sum_{\gamma} m_{\gamma}\ddot{\mathbf{u}}_{\gamma} = \sum_{\alpha}\sum_{\beta,\gamma}\mathbf{F}^{\gamma}_{\alpha\beta} + \sum_{\gamma}\mathbf{f}^{*}_{\gamma}, \quad \sum_{\gamma}\boldsymbol{\theta}_{\gamma}\cdot\ddot{\boldsymbol{\varphi}}_{\gamma} = \sum_{\alpha}\sum_{\beta,\gamma}\mathbf{M}^{\gamma}_{\alpha\beta} + \sum_{\gamma}\mathbf{m}^{*}_{\gamma} \tag{3.2}$$

are a corollary of Eq. (3.1).

We shall henceforth refer to Eq. (3.2) as the equations of motion of the initial cell. Note, however, that Eq. (3.2) are obtained by formal summation of Eq. (3.1). Here, the first equation is actually a formulation of Euler's first law of dynamics and the second equation, strictly speaking, is not a formulation of Euler's second law of dynamics for the initial cell.

4. Description of the interaction of the lattice particles

We will now consider two interacting particles: the particle γ of the initial cell, the position of which is defined by the vector $\mathbf{r}_{\gamma}$, and the particle β of the cell -α, the position of which is defined by the vector $\mathbf{r}_{\beta} - \mathbf{a}_{\alpha}$, a force $\mathbf{F}^{\gamma}_{-\alpha\beta}(\mathbf{r}_{\gamma})$ and a moment $\mathbf{M}^{\gamma}_{-\alpha\beta}(\mathbf{r}_{\gamma})$ (the moment is calculated with reference to particle γ in the initial cell) act on particle γ of the initial cell on the part of particle β in the cell -α. With respect to the cell -α, the initial cell is cell α. Consequently, a force $\mathbf{F}^{\beta}_{\alpha\gamma}(\mathbf{r}_{\beta} - \mathbf{a}_{\alpha})$ and a moment $\mathbf{M}^{\beta}_{\alpha\gamma}(\mathbf{r}_{\beta} - \mathbf{a}_{\alpha})$ (the moment is calculated with reference to particle β of the cell -α) act on particle β of the cell -α on the part of the particle γ of the initial cell. According to Newton's third law for forces and its analogue for moments (1.6), the following relations hold (see Fig. 2)

$$\begin{aligned}&\mathbf{F}^{\gamma}_{-\alpha\beta}(\mathbf{r}_{\gamma}) + \mathbf{F}^{\beta}_{\alpha\gamma}(\mathbf{r}_{\beta} - \mathbf{a}_{\alpha}) = 0\\ &\mathbf{M}^{\gamma}_{-\alpha\beta}(\mathbf{r}_{\gamma}) - \frac{1}{2}\mathbf{a}^{\gamma}_{-\alpha\beta}\times\mathbf{F}^{\gamma}_{-\alpha\beta}(\mathbf{r}_{\gamma}) + \mathbf{M}^{\beta}_{\alpha\gamma}(\mathbf{r}_{\beta} - \mathbf{a}_{\alpha}) - \frac{1}{2}\mathbf{a}^{\beta}_{\alpha\gamma}\times\mathbf{F}^{\beta}_{\alpha\gamma}(\mathbf{r}_{\beta} - \mathbf{a}_{\alpha}) = 0\end{aligned} \tag{4.1}$$

We shall assume that $\mathbf{F}^{\beta}_{\alpha\gamma}$ and $\mathbf{M}^{\beta}_{\alpha\gamma}$ are not only defined for a discrete set of values $\mathbf{r}_{\beta} \pm \mathbf{a}_{\alpha}$ but, also, for the continuous set $\mathbf{r}$, where $\mathbf{r}$ defines the position of an arbitrary point of space. As the definitions of the functions $\mathbf{F}^{\beta}_{\alpha\gamma}(\mathbf{r})$ and $\mathbf{M}^{\beta}_{\alpha\gamma}(\mathbf{r})$ are just extended, it does not change their meaning. However, it is important that these functions should be differentiable and only vary slightly within an interval of the order of interatomic interactions.

Assuming that the long-wave approximation holds (see Ref 7), we have

$$\mathbf{F}^{\beta}_{\alpha\gamma}(\mathbf{r}_{\beta} - \mathbf{a}_{\alpha}) \approx \mathbf{F}^{\beta}_{\alpha\gamma}(\mathbf{r}_{\beta}) - \mathbf{a}_{\alpha}\cdot\nabla_{\beta}\mathbf{F}^{\beta}_{\alpha\gamma}, \quad \mathbf{M}^{\beta}_{\alpha\gamma}(\mathbf{r}_{\beta} - \mathbf{a}_{\alpha}) \approx \mathbf{M}^{\beta}_{\alpha\gamma}(\mathbf{r}_{\beta}) - \mathbf{a}_{\alpha}\cdot\nabla_{\beta}\mathbf{M}^{\beta}_{\alpha\gamma} \tag{4.2}$$

where ∇_β is the operator ∇, calculated at a point of the initial cell, the position of which is defined by the vector $\mathbf{r}_\beta$. The relations

$$\begin{aligned}\mathbf{F}^\gamma_{-\alpha\beta}(\mathbf{r}_\gamma) &\approx -\mathbf{F}^\beta_{\alpha\gamma}(\mathbf{r}_\beta) + \mathbf{a}_\alpha \cdot \nabla_\beta \cdot \mathbf{F}^\beta_{\alpha\gamma} \\ \mathbf{M}^\gamma_{-\alpha\beta}(\mathbf{r}_\gamma) &\approx -\mathbf{M}^\beta_{\alpha\gamma}(\mathbf{r}_\beta) + \mathbf{a}^\beta_{\alpha\gamma} \times \mathbf{F}^\beta_{\alpha\gamma}(\mathbf{r}_\beta) + \mathbf{a}_\alpha \nabla_\beta \cdot \hat{\mathbf{M}}^\beta_{\alpha\gamma}\end{aligned} \tag{4.3}$$

where $\hat{\mathbf{M}}^\beta_{\alpha\beta} = \mathbf{M}^\beta_{\alpha\beta} - \mathbf{a}^\beta_{\alpha\beta} \times \mathbf{F}^\beta_{\alpha\beta}$ is a vector having the sense of the moment acting on particle β of the initial cell on the part of particle γ of the cell α, calculated with reference to particle γ of cell α, are a corollary of formulae (4.1) and (4.2). Using formulae (4.3), we carry out the following transformations

$$\begin{aligned}\sum_\alpha \sum_{\beta,\gamma} \mathbf{F}^\gamma_{\alpha\beta} &= \frac{1}{2} \sum_{\alpha,\beta,\gamma} (\mathbf{F}^\gamma_{\alpha\beta} + \mathbf{F}^\gamma_{-\alpha\beta}) \approx \nabla \cdot \left(\frac{1}{2} \sum_{\alpha,\beta,\gamma} \mathbf{a}_\alpha \mathbf{F}^\beta_{\alpha\gamma} \right) \\ \sum_\alpha \sum_{\beta,\gamma} \mathbf{M}^\gamma_{\alpha\beta} &= \frac{1}{2} \sum_{\alpha,\beta,\gamma} (\mathbf{M}^\gamma_{\alpha\beta} + \mathbf{M}^\gamma_{-\alpha\beta}) \approx \left(\frac{1}{2} \sum_{\alpha,\beta,\gamma} \mathbf{a}^\beta_{\alpha\gamma} \mathbf{F}^\beta_{\alpha\gamma} \right)_\times + \nabla \cdot \left(\frac{1}{2} \sum_{\alpha,\beta,\gamma} \mathbf{a}_\alpha \hat{\mathbf{M}}^\beta_{\alpha\gamma} \right)\end{aligned} \tag{4.4}$$

The sign $()_\times$ is the notation for a vector invariant. In formulae (4.4), the approximation $\nabla_\beta \approx \nabla$ is used and the operator ∇ is calculated at a point of the initial cell, the position of which is defined by the vector $\mathbf{r}$. Note that, on transferring to the long-wave approximation, the vector $\mathbf{r}$ can be considered as the vector defining the position of the initial cell. When account is taken of relations (4.4), the equations of motion of the initial cell (3.2) in the log-wave approximation are written as

$$\begin{aligned}\sum_\gamma m_\gamma \ddot{\mathbf{u}}_\gamma &= \nabla \cdot \left(\frac{1}{2} \sum_{\alpha,\beta,\gamma} \mathbf{a}_\alpha \mathbf{F}^\beta_{\alpha\gamma} \right) + \sum_\gamma \mathbf{f}^*_\gamma \\ \sum_\gamma \boldsymbol{\theta}_\gamma \cdot \ddot{\boldsymbol{\varphi}}_\gamma &= \left(\frac{1}{2} \sum_{\alpha,\beta,\gamma} \mathbf{a}^\beta_{\alpha\gamma} \mathbf{F}^\beta_{\alpha\gamma} \right)_\times + \nabla \cdot \left(\frac{1}{2} \sum_{\alpha,\beta,\gamma} \mathbf{a}_\alpha \hat{\mathbf{M}}^\beta_{\alpha\gamma} \right) + \sum_\gamma \mathbf{m}^*_\gamma\end{aligned} \tag{4.5}$$

The differential equations of motion of the initial cell are thereby obtained.

It will be shown below that, with a corresponding definition of the concepts of stress tensors, vectors for the bulk density of external loads and displacement vectors, the differential Eq. (4.5) are identical to the equations of motion of a macroscopic moment theory of elasticity.

5. Internal equilibrium equations

Differential Eq. (4.5) describe the motion of the unit cell as a whole and do not characterize the individual motions of each of the particles. The motions of each particle in a unit cell are described by Eq. (3.1). However, since only the asymptotically principal terms are retained in the equations of motion of the cell (4.5), it also makes sense to discard the correction terms in the equations of the particles (3.1).

Hence, we will carry out a non-rigorous asymptotic analysis of the equations of motion of the particles of the initial cell (3.1). We take the quantity $\mathbf{a}_\alpha \cdot \nabla \sim \varepsilon$ as a small parameter and assume here that $\varepsilon M \ll 1$, where M is the number of particles in the unit cell. Then, when account is taken of the identity

$$\sum_{\alpha,\beta,\gamma} \mathbf{a}^\beta_{\alpha\gamma} \times \mathbf{F}^\beta_{\alpha\gamma} = \sum_{\alpha,\beta,\gamma} \mathbf{a}^\gamma_{\alpha\beta} \times \mathbf{F}^\gamma_{\alpha\beta}$$

the following asymptotic estimates can be obtained from Eq. (4.5)

$$\sum_\gamma m_\gamma \ddot{\mathbf{u}}_\gamma - \sum_\gamma \mathbf{f}^*_\gamma \sim \varepsilon M^2 \mathbf{F}^\gamma_{\alpha\beta}, \quad \sum_\gamma \boldsymbol{\theta}_\gamma \cdot \ddot{\boldsymbol{\varphi}}_\gamma - \sum_\gamma \mathbf{m}^*_\gamma - \frac{1}{2} \sum_{\alpha,\beta,\gamma} \mathbf{a}^\gamma_{\alpha\beta} \times \mathbf{F}^\gamma_{\alpha\beta} \sim \varepsilon M^2 \mathbf{M}^\gamma_{\alpha\beta} \tag{5.1}$$

We will assume that the external loads are slowly varying functions of the spatial coordinates, that is,

$$\left|\mathbf{f}_\gamma^* - \mathbf{f}_\beta^*\right| \sim \varepsilon\left|\mathbf{f}_\gamma^*\right|, \quad \left|\mathbf{m}_\gamma^* - \mathbf{m}_\beta^*\right| \sim \varepsilon\left|\mathbf{m}_\gamma^*\right|$$

It will be shown below that the asymptotic estimates

$$\left|\mathbf{u}_\gamma - \mathbf{u}_\beta\right| \sim \varepsilon\left|\mathbf{u}_\gamma\right|, \quad \left|\boldsymbol{\varphi}_\gamma - \boldsymbol{\varphi}_\beta\right| \sim \varepsilon\left|\boldsymbol{\varphi}_\gamma\right| \tag{5.2}$$

hold for the displacements and rotations of the particles in a cell.

Consequently,

$$\sum_\gamma (m_\gamma \ddot{\mathbf{u}}_\gamma - \mathbf{f}_\gamma^*) \approx M(m_\gamma \ddot{\mathbf{u}}_\gamma - \mathbf{f}_\gamma^*), \quad \sum_\gamma (\boldsymbol{\theta}_\gamma \cdot \ddot{\boldsymbol{\varphi}}_\gamma - \mathbf{m}_\gamma^*) \approx M(\boldsymbol{\theta}_\gamma \cdot \ddot{\boldsymbol{\varphi}}_\gamma - \mathbf{m}_\gamma^*)$$

Then, in accordance with estimates (5.1), it can be confirmed that

$$m_\gamma \ddot{\mathbf{u}}_\gamma - \mathbf{f}_\gamma^* \sim \varepsilon M \mathbf{F}_{\alpha\beta}^\gamma, \quad \boldsymbol{\theta}_\gamma \cdot \ddot{\boldsymbol{\varphi}}_\gamma - \mathbf{m}_\gamma^* - \frac{1}{2}\sum_{\alpha,\,\beta} \mathbf{a}_{\alpha\beta}^\gamma \times \mathbf{F}_{\alpha\beta}^\gamma \sim \varepsilon M \mathbf{M}_{\alpha\beta}^\gamma \tag{5.3}$$

Consequently, the asymptotically principal terms of Eq. (3.1) have the form

$$\sum_{\alpha,\,\beta} \mathbf{F}_{\alpha\beta}^\gamma = 0, \quad \sum_{\alpha,\,\beta}\left(\mathbf{M}_{\alpha\beta}^\gamma - \frac{1}{2}\mathbf{a}_{\alpha\beta}^\gamma \times \mathbf{F}_{\alpha\beta}^\gamma\right) = 0 \tag{5.4}$$

Thus, $2M$ internal equilibrium equations have been obtained. The equations of the first group are the force balance equations but the equations of the second group are not, strictly speaking, moment balance equations since they are the sum of moments calculated with reference to different points. Note that there are only $2(M-1)$ independent equations among Eq. (5.4). In fact, using the asymptotically principal terms of relations (4.4), it is easy to show that $\sum_\gamma$ of Eq. (5.4) are identically equal to zero. This confirms the correctness of Eq. (5.4).

Note that the important identities

$$\sum_{\alpha,\,\beta,\,\gamma} \mathbf{a}_\alpha \mathbf{F}_{\alpha\gamma}^\beta = \sum_{\alpha,\,\beta,\,\gamma} \mathbf{a}_{\alpha\gamma}^\beta \mathbf{F}_{\alpha\gamma}^\beta, \quad \sum_{\alpha,\,\beta,\,\gamma} \mathbf{a}_\alpha \hat{\mathbf{M}}_{\alpha\gamma}^\beta = \sum_{\alpha,\,\beta,\,\gamma} \mathbf{a}_{\alpha\gamma}^\beta \hat{\mathbf{M}}_{\alpha\gamma}^\beta \tag{5.5}$$

can be proved using Eq. (5.4). It is also easy to shown that the following identities hold

$$\sum_{\alpha,\,\beta,\,\gamma} \mathbf{a}_\alpha \mathbf{a}_{\alpha\gamma}^\beta \times \mathbf{F}_{\alpha\gamma}^\beta = 0, \quad \sum_{\alpha,\,\beta,\,\gamma} \mathbf{a}_{\alpha\gamma}^\beta \mathbf{a}_{\alpha\gamma}^\beta \times \mathbf{F}_{\alpha\gamma}^\beta = 0 \tag{5.6}$$

6. The continual equations of motion

By taking account of identities (5.5) and (5.6), it can be shown that the equations of motion of the initial cell (4.5) are identical to the equation for the dynamics of a macroscopic moment theory of elasticity

$$\nabla \cdot \boldsymbol{\tau} + \mathbf{f} = \rho \ddot{\mathbf{u}}, \quad \nabla \cdot \boldsymbol{\mu} + \boldsymbol{\tau}_\times + \mathbf{m} = \rho \boldsymbol{\vartheta} \cdot \ddot{\boldsymbol{\varphi}} \tag{6.1}$$

The equivalence of Eqs. (4.5) and (6.1) is achieved using the following notation

$$\boldsymbol{\tau} = \frac{1}{2V_*}\sum_{\alpha,\,\beta,\,\gamma} \mathbf{a}_{\alpha\gamma}^\beta \mathbf{F}_{\alpha\gamma}^\beta, \quad \boldsymbol{\mu} = \frac{1}{2V_*}\sum_{\alpha,\,\beta,\,\gamma} \mathbf{a}_{\alpha\gamma}^\beta \left[\mathbf{M}_{\alpha\gamma}^\beta - \frac{1}{2}\mathbf{a}_{\alpha\gamma}^\beta \times \mathbf{F}_{\alpha\gamma}^\beta\right] \tag{6.2}$$

$$\left(\sum_\gamma m_\gamma\right)\mathbf{u} = \sum_\gamma m_\gamma \mathbf{u}_\gamma, \quad \left(\sum_\gamma \boldsymbol{\theta}_\gamma\right) \cdot \boldsymbol{\varphi} = \sum_\gamma \boldsymbol{\theta}_\gamma \cdot \boldsymbol{\varphi}_\gamma \tag{6.3}$$

$$\rho = \frac{1}{V_*}\sum_\gamma m_\gamma, \quad \rho\vartheta = \frac{1}{V_*}\sum_\gamma \boldsymbol{\theta}_\gamma, \quad \mathbf{f} = \frac{1}{V_*}\sum_\gamma \mathbf{f}^*_\gamma, \quad \mathbf{m} = \frac{1}{V_*}\sum_\gamma \mathbf{m}^*_\gamma \tag{6.4}$$

Here, V_* is the volume of a unit cell. We shall call the tensor $\boldsymbol{\tau}$ the stress tensor, and the tensor $\boldsymbol{\mu}$ is the stress moment tensor. The vector $\mathbf{u}$ determines the displacement of the centre of mass of the initial cell (we shall refer to it as the cell displacement vector), the vector $\boldsymbol{\varphi}$ is the rotation vector averaged over the particles (we shall refer to it as the cell rotation vector), ρ is the mass density, ϑ is the inertial tensor of the medium per unit mass (or the mass density of the inertial tensor), $\mathbf{f}$ is the bulk density of the external forces and $\mathbf{m}$ is the bulk density of the external moments.

We will rewrite the internal equilibrium Eq. (5.4) in the form

$$\sum_\beta \boldsymbol{\tau}^\gamma_\beta = 0, \quad \sum_\beta \boldsymbol{\mu}^\gamma_\beta = 0 \tag{6.5}$$

where the notation

$$\boldsymbol{\tau}^\gamma_\beta = \frac{1}{2V_*}\sum_\alpha \mathbf{F}^\gamma_{\alpha\beta}, \quad \boldsymbol{\mu}^\gamma_\beta = \frac{1}{2V_*}\sum_\alpha \left(\mathbf{M}^\gamma_{\alpha\beta} - \frac{1}{2}\mathbf{a}^\gamma_{\alpha\beta}\times\mathbf{F}^\gamma_{\alpha\beta}\right) \tag{6.6}$$

has been introduced. We shall call the vector $\boldsymbol{\tau}^\gamma_\beta$ the stress vector and the vector $\boldsymbol{\mu}^\gamma_\beta$ the stress moment vector.

Eqs. (6.1) and (6.5) are the continual equations of motion of a cell with a microstructure.

7. Strain tensors and discrepancy vectors

We will consider two interacting particles: the particle γ of the initial cell and the particle β in the cell α. The strain vectors of this systems $\boldsymbol{\varepsilon}^\gamma_{\alpha\beta}$, $\boldsymbol{\kappa}^\gamma_{\alpha\beta}$ are defined by formula (1.12) and have the form

$$\boldsymbol{\varepsilon}^\gamma_{\alpha\beta} = \mathbf{u}_\beta(\mathbf{r}_\beta + \mathbf{a}_\alpha) - \mathbf{u}_\gamma(\mathbf{r}_\gamma) + \mathbf{a}^\gamma_{\alpha\beta}\times\boldsymbol{\varphi}_\beta(\mathbf{r}_\beta + \mathbf{a}_\alpha), \quad \boldsymbol{\kappa}^\gamma_{\alpha\beta} = \boldsymbol{\varphi}_\beta(\mathbf{r}_\beta + \mathbf{a}_\alpha) - \boldsymbol{\varphi}_\gamma(\mathbf{r}_\gamma) \tag{7.1}$$

Using the long-wave approximation (see Ref 7), we write the expressions for the strain vectors (7.1)

$$\boldsymbol{\varepsilon}^\gamma_{\alpha\beta} = \mathbf{a}^\gamma_{\alpha\beta}\cdot\boldsymbol{\varepsilon} + \mathbf{u}^\gamma_\beta + \frac{1}{2}\mathbf{a}^\gamma_{\alpha\beta}\times(\mathbf{a}^\gamma_{\alpha\beta}\cdot\boldsymbol{\kappa} + \boldsymbol{\varphi}^\gamma_\beta), \quad \boldsymbol{\kappa}^\gamma_{\alpha\beta} = \mathbf{a}^\gamma_{\alpha\beta}\cdot\boldsymbol{\kappa} + \boldsymbol{\varphi}^\gamma_\beta \tag{7.2}$$

Here, the lattice strain tensors

$$\boldsymbol{\varepsilon} = \frac{1}{2}\nabla_\gamma(\mathbf{u}_\beta + \mathbf{u}_\gamma) + \mathbf{E}\times\frac{1}{2}[\boldsymbol{\varphi}_\beta + \boldsymbol{\varphi}_\gamma] \quad \boldsymbol{\kappa} = \frac{1}{2}\nabla_\gamma(\boldsymbol{\varphi}_\beta + \boldsymbol{\varphi}_\gamma) \tag{7.3}$$

are introduced into the treatment, where $\mathbf{E}$ is a unit tensor, and the discrepancy vectors

$$\mathbf{u}^\gamma_\beta = \mathbf{u}_\beta - \mathbf{u}_\gamma, \quad \boldsymbol{\varphi}^\gamma_\beta = \boldsymbol{\varphi}_\beta - \boldsymbol{\varphi}_\gamma \tag{7.4}$$

All the quantities in formulae (7.3) and (7.4) are calculated when $\mathbf{r} = \mathbf{r}_\gamma + \mathbf{a}^\gamma_{\alpha\beta}/2$.

Note that, according to estimates (5.2), the justification for which will be given below, and formulae (6.3), which introduce the displacement and cell rotation vectors $\mathbf{u}$ and $\boldsymbol{\varphi}$ into the treatment, the approximations

$$\mathbf{u}_\gamma \approx \mathbf{u}, \quad \boldsymbol{\varphi}_\gamma \approx \boldsymbol{\varphi}$$

hold, which permit an error $O(\varepsilon)$ in comparison with the leading term. The strain tensors (7.3) can then be rewritten in the form

$$\boldsymbol{\varepsilon} = \nabla\mathbf{u} + \mathbf{E}\times\boldsymbol{\varphi}, \quad \boldsymbol{\kappa} = \nabla\boldsymbol{\varphi} \tag{7.5}$$

The asymptotically leading terms of expressions (7.3) and (7.5) are therefore identical.

8. The elasticity relations in implicit form

Consider two interacting particles: the particle γ of the initial cell and the particle β in the cell α, According to formulae (1.12), the elasticity relations for the system of particles being considered have the form

$$\mathbf{F}^{\gamma}_{\alpha\beta} = \tilde{\mathbf{F}}^{\gamma}_{\alpha\beta} + \tilde{\mathbf{A}}^{\gamma}_{\alpha\beta}\cdot\boldsymbol{\varepsilon}^{\gamma}_{\alpha\beta} + \mathbf{B}^{\gamma}_{\alpha\beta}\cdot\boldsymbol{\kappa}^{\gamma}_{\alpha\beta}, \quad \mathbf{M}^{\gamma}_{\alpha\beta} = \tilde{\mathbf{M}}^{\gamma}_{\alpha\beta} + \boldsymbol{\varepsilon}^{\gamma}_{\alpha\beta}\cdot\tilde{\mathbf{B}}^{\gamma}_{\alpha\beta} + \tilde{\mathbf{C}}^{\gamma}_{\alpha\beta}\cdot\boldsymbol{\kappa}^{\gamma}_{\alpha\beta} \tag{8.1}$$

Substituting expressions (7.2) into elasticity relations (8.1) and using the relations for the stiffness tensors (1.13), after some reduction we obtain expressions for the force and moment vectors in the form of functions of the strain tensors and the discrepancy vectors. On substituting them into formulae (6.2) and (6.6), we obtain the expressions for the stress tensors and vectors

$$\begin{aligned}
&\boldsymbol{\tau} = \boldsymbol{\tau}_0 + {}^4\mathbf{A}^{*}\cdot\cdot\,\boldsymbol{\varepsilon} + {}^4\mathbf{B}^{*}\cdot\cdot\,\boldsymbol{\kappa} + \sum_{\beta,\gamma}[{}^3\mathbf{A}^{\gamma}_{\beta}\cdot\mathbf{u}^{\gamma}_{\beta} + {}^3\mathbf{B}^{\gamma}_{\beta}\cdot\boldsymbol{\varphi}^{\gamma}_{\beta}]\\
&\boldsymbol{\mu} = \boldsymbol{\mu}_0 + ({}^4\mathbf{B}^{*})^{T}\cdot\cdot\,\boldsymbol{\varepsilon} + {}^4\mathbf{C}^{*}\cdot\cdot\,\boldsymbol{\kappa} + \sum_{\beta,\gamma}[({}^3\mathbf{B}^{\gamma}_{\beta})^{t}\cdot\mathbf{u}^{\gamma}_{\beta} + {}^3\mathbf{C}^{\gamma}_{\beta}\cdot\boldsymbol{\varphi}^{\gamma}_{\beta}]\\
&\boldsymbol{\tau}^{\gamma}_{\beta} = \tilde{\boldsymbol{\tau}}^{\gamma}_{\beta} + \boldsymbol{\varepsilon}^{T}\cdot\cdot\,{}^3\mathbf{A}^{\gamma}_{\beta} + \boldsymbol{\kappa}^{T}\cdot\cdot\,({}^3\mathbf{B}^{\gamma}_{\beta})^{t} + \mathbf{A}^{\gamma}_{\beta}\cdot\mathbf{u}^{\gamma}_{\beta} + \mathbf{B}^{\gamma}_{\beta}\cdot\boldsymbol{\varphi}^{\gamma}_{\beta}\\
&\boldsymbol{\mu}^{\gamma}_{\beta} = \tilde{\boldsymbol{\mu}}^{\gamma}_{\beta} + \boldsymbol{\varepsilon}^{T}\cdot\cdot\,{}^3\mathbf{B}^{\gamma}_{\beta} + \boldsymbol{\kappa}^{T}\cdot\cdot\,{}^3\mathbf{C}^{\gamma}_{\beta} + ({}^3\mathbf{B}^{\gamma}_{\beta})^{T}\cdot\mathbf{u}^{\gamma}_{\beta} + \mathbf{C}^{\gamma}_{\beta}\cdot\boldsymbol{\varphi}^{\gamma}_{\beta}
\end{aligned} \tag{8.2}$$

The stiffness tensors are calculated using the formulae

$$\begin{aligned}
&{}^4\mathbf{Z}^{*} = \frac{1}{2V_*}\sum_{\alpha,\beta,\gamma}\mathbf{a}^{\gamma}_{\alpha\beta}\mathbf{Z}^{\gamma}_{\alpha\beta}\mathbf{a}^{\gamma}_{\alpha\beta}, \quad {}^3\mathbf{Z}^{\gamma}_{\beta} = \frac{1}{2V_*}\sum_{\alpha}\mathbf{a}^{\gamma}_{\alpha\beta}\mathbf{Z}^{\gamma}_{\alpha\beta}, \quad \mathbf{Z}^{\gamma}_{\beta} = \frac{1}{2V_*}\sum_{\alpha}\mathbf{Z}^{\gamma}_{\alpha\beta}, \quad \mathbf{Z} = \mathbf{A},\mathbf{B},\mathbf{C}\\
&({}^4\mathbf{B}^{*})^{T} = \frac{1}{2V_*}\sum_{\alpha,\beta,\gamma}\mathbf{a}^{\gamma}_{\alpha\beta}(\mathbf{B}^{\gamma}_{\alpha\beta})^{T}\mathbf{a}^{\gamma}_{\alpha\beta}, \quad ({}^3\mathbf{B}^{\gamma}_{\beta})^{t} = \frac{1}{2V_*}\sum_{\alpha}\mathbf{a}^{\gamma}_{\alpha\beta}(\mathbf{B}^{\gamma}_{\alpha\beta})^{T}\\
&\boldsymbol{\tau}_0 = \frac{1}{2V_*}\sum_{\alpha,\beta,\gamma}\mathbf{a}^{\gamma}_{\alpha\beta}\tilde{\mathbf{F}}^{\gamma}_{\alpha\beta}, \quad \boldsymbol{\mu}_0 = \frac{1}{2V_*}\sum_{\alpha,\beta,\gamma}\mathbf{a}^{\gamma}_{\alpha\beta}\left(\tilde{\mathbf{M}}^{\gamma}_{\alpha\beta} - \frac{1}{2}\mathbf{a}^{\gamma}_{\alpha\beta}\times\tilde{\mathbf{F}}^{\gamma}_{\alpha\beta}\right)\\
&\tilde{\boldsymbol{\tau}}^{\gamma}_{\beta} = \frac{1}{2V_*}\sum_{\alpha}\tilde{\mathbf{F}}^{\gamma}_{\alpha\beta}, \quad \tilde{\boldsymbol{\mu}}^{\gamma}_{\beta} = \frac{1}{2V_*}\sum_{\alpha}\left(\tilde{\mathbf{M}}^{\gamma}_{\alpha\beta} - \frac{1}{2}\mathbf{a}^{\gamma}_{\alpha\beta}\times\tilde{\mathbf{F}}^{\gamma}_{\alpha\beta}\right)
\end{aligned} \tag{8.3}$$

Hence, formulae (8.2) enable us to express the stress tensors and vectors in terms of the lattice strain tensors $\boldsymbol{\varepsilon}$ and $\boldsymbol{\kappa}$ and the discrepancy vectors $\mathbf{u}^{\gamma}_{\beta}$, $\boldsymbol{\varphi}^{\gamma}_{\beta}$. The internal equilibrium Eq. (6.5) serve to determine the relation between the discrepancy vectors and the lattice strain tensors. On substituting the expressions for the stress vectors (8.2) into Eq. (6.5), we obtain the system of $2M$ equations (of which $2(M-1)$ are independent)

$$\begin{aligned}
&\boldsymbol{\varepsilon}^{T}\cdot\cdot\,{}^3\mathbf{A}^{\gamma} + \boldsymbol{\kappa}^{T}\cdot\cdot\,({}^3\mathbf{B}^{\gamma})^{t} + \sum_{\beta}[\mathbf{A}^{\gamma}_{\beta}\cdot\mathbf{u}^{\gamma}_{\beta} + \mathbf{B}^{\gamma}_{\beta}\cdot\boldsymbol{\varphi}^{\gamma}_{\beta}] = 0\\
&\boldsymbol{\varepsilon}^{T}\cdot\cdot\,{}^3\mathbf{B}^{\gamma} + \boldsymbol{\kappa}^{T}\cdot\cdot\,{}^3\mathbf{C}^{\gamma} + \sum_{\beta}[(\mathbf{B}^{\gamma}_{\beta})^{T}\cdot\mathbf{u}^{\gamma}_{\beta} + \mathbf{C}^{\gamma}_{\beta}\cdot\boldsymbol{\varphi}^{\gamma}_{\beta}] = 0
\end{aligned} \tag{8.4}$$

The second-rank stiffness tensors are defined by expressions (8.3) and the third-rank stiffness tensors are calculated using the formulae

$${}^3\mathbf{A}^{\gamma} = \sum_{\beta}{}^3\mathbf{A}^{\gamma}_{\beta}, \quad {}^3\mathbf{B}^{\gamma} = \sum_{\beta}{}^3\mathbf{B}^{\gamma}_{\beta}, \quad {}^3\mathbf{C}^{\gamma} = \sum_{\beta}{}^3\mathbf{C}^{\gamma}_{\beta} \tag{8.5}$$

In deriving Eq. (8.4), account has been taken of the fact that the equilibrium conditions of the reference configuration

$$\sum_\beta \tilde{\tau}_\beta^\gamma = 0, \quad \sum_\beta \tilde{\mu}_\beta^\gamma = 0 \tag{8.6}$$

are satisfied in the case of the initial stresses.

Taking the expressions for the discrepancy vectors (7.4) into account, we note that system (8.4) is actually a system of equations in the displacement vectors and the rotation vectors $\mathbf{u}_\gamma$, $\boldsymbol{\varphi}_\gamma$.

9. The elasticity relations in explicit form

We will now represent the displacement and rotation vectors in the form

$$\mathbf{u}_\gamma = \boldsymbol{\varepsilon}^T \cdot\cdot\, {}^3\mathbf{U}_\gamma^\varepsilon + \boldsymbol{\kappa}^T \cdot\cdot\, {}^3\mathbf{U}_\gamma^\kappa + \mathbf{u}_0, \quad \boldsymbol{\varphi}_\gamma = \boldsymbol{\varepsilon}^T \cdot\cdot\, {}^3\boldsymbol{\Phi}_\gamma^\varepsilon + \boldsymbol{\kappa}^T \cdot\cdot\, {}^3\boldsymbol{\Phi}_\gamma^\kappa + \boldsymbol{\varphi}_0 \tag{9.1}$$

We shall call the third rank tensors ${}^3\mathbf{U}_\gamma^\varepsilon$, ${}^3\mathbf{U}_\gamma^\kappa$, ${}^3\Phi\gamma\varepsilon$, ${}^3\Phi\gamma\kappa$ the internal bond tensors and note that the vectors $\mathbf{u}_\gamma$, $\boldsymbol{\varphi}_\gamma$ can always be represented in the form (9.1), since this is a general linear relation between the vectors $\mathbf{u}_\gamma$, $\boldsymbol{\varphi}_\gamma$ and the second-rank tensors $\boldsymbol{\varepsilon}$ and $\boldsymbol{\kappa}$. Substituting expressions (9.1) into the relations for the discrepancy vectors (7.4), we obtain

$$\begin{aligned} \mathbf{u}_\beta^\gamma &= \boldsymbol{\varepsilon}^T \cdot\cdot\, ({}^3\mathbf{U}_\beta^\varepsilon - {}^3\mathbf{U}_\gamma^\varepsilon) + \boldsymbol{\kappa}^T \cdot\cdot\, ({}^3\mathbf{U}_\beta^\kappa - {}^3\mathbf{U}_\gamma^\kappa) \\ \boldsymbol{\varphi}_\beta^\gamma &= \boldsymbol{\varepsilon}^T \cdot\cdot\, ({}^3\boldsymbol{\Phi}_\beta^\varepsilon - {}^3\boldsymbol{\Phi}_\gamma^\varepsilon) + \boldsymbol{\kappa}^T \cdot\cdot\, ({}^3\boldsymbol{\Phi}_\beta^\kappa - {}^3\boldsymbol{\Phi}_\gamma^\kappa) \end{aligned} \tag{9.2}$$

Note that the expressions for the discrepancy vectors (7.4) are independent of the vectors $\mathbf{u}_0$ and $\boldsymbol{\varphi}_0$. Consequently, the vectors $\mathbf{u}_0$ and $\boldsymbol{\varphi}_0$ can be chosen arbitrarily. It should be possible to equate them to zero but it is more convenient to define them as follows:

$$\sum_\gamma \mathbf{u}_\gamma = M\mathbf{u}_0, \quad \sum_\gamma \boldsymbol{\varphi}_\gamma = M\boldsymbol{\varphi}_0 \tag{9.3}$$

We will now obtain the equations for determining the internal bond tensors. To do this, we substitute the expressions for the discrepancy vectors (9.2) into Eq. (8.4), which leads to a system of linear homogeneous algebraic equations in the strain tensors. The equations must hold for any values of the strain tensors. This is possible if the coefficients accompanying the strain tensors are identically equal to zero. On equating the coefficients accompanying the tensors $\boldsymbol{\varepsilon}$ and $\boldsymbol{\kappa}$ to zero, we obtain a system of $4M$ equations for the internal bond tensors, of which only $4(M-1)$ are independent. In order to close this system of equations, we note that the two linear homogeneous equations, which are geometric relations, are a corollary of relations (9.1) and (9.3). Since these equations must be satisfied for any $\boldsymbol{\varepsilon}$ and $\boldsymbol{\kappa}$, they are equivalent to four equations which superimpose the geometric relations on the internal bond tensors. The addition of these equations to the system obtained earlier gives a closed system of $4M$ equations in the internal bond tensors which decomposes into two independent systems of $2M$ equations

$$\begin{aligned} &{}^3\mathbf{A}^\gamma + \sum_\beta [{}^3\mathbf{U}_\beta^\varepsilon - {}^3\mathbf{U}_\gamma^\varepsilon] \cdot \mathbf{A}_\beta^\gamma + \sum_\beta [{}^3\boldsymbol{\Phi}_\beta^\varepsilon - {}^3\boldsymbol{\Phi}_\gamma^\varepsilon] \cdot (\mathbf{B}_\beta^\gamma)^T = 0, \quad \sum_\gamma {}^3\mathbf{U}_\gamma^\varepsilon = 0 \\ &{}^3\mathbf{B}^\gamma + \sum_\beta [{}^3\mathbf{U}_\beta^\varepsilon - {}^3\mathbf{U}_\gamma^\varepsilon] \cdot \mathbf{B}_\beta^\gamma + \sum_\beta [{}^3\boldsymbol{\Phi}_\beta^\varepsilon - {}^3\boldsymbol{\Phi}_\gamma^\varepsilon] \cdot \mathbf{C}_\beta^\gamma = 0, \quad \sum_\gamma {}^3\boldsymbol{\Phi}_\gamma^\varepsilon = 0 \\ &({}^3\mathbf{B}^\gamma)^t + \sum_\beta [{}^3\mathbf{U}_\beta^\kappa - {}^3\mathbf{U}_\gamma^\kappa] \cdot \mathbf{A}_\beta^\gamma + \sum_\beta [{}^3\boldsymbol{\Phi}_\beta^\kappa - {}^3\boldsymbol{\Phi}_\gamma^\kappa] \cdot (\mathbf{B}_\beta^\gamma)^T = 0, \quad \sum_\gamma {}^3\mathbf{U}_\gamma^\kappa = 0 \\ &{}^3\mathbf{C}^\gamma + \sum_\beta [{}^3\mathbf{U}_\beta^\kappa - {}^3\mathbf{U}_\gamma^\kappa] \cdot \mathbf{B}_\beta^\gamma + \sum_\beta [{}^3\boldsymbol{\Phi}_\beta^\kappa - {}^3\boldsymbol{\Phi}_\gamma^\kappa] \cdot \mathbf{C}_\beta^\gamma = 0, \quad \sum_\gamma {}^3\boldsymbol{\Phi}_\gamma^\kappa = 0 \end{aligned} \tag{9.4}$$

As can be seen from Eq. (9.4), the internal bond tensors are characteristics of the material and are independent of the motion of the lattice particles. Note that it follows from formulae (9.1) for the displacements $\mathbf{u}_\gamma$ and the rotations

$\boldsymbol{\varphi}_\gamma$, where the internal bond tensors are defined by Eq. (9.4), that $|\mathbf{u}_\gamma - \mathbf{u}|$ is a small quantity of the order of $\varepsilon\mathbf{u}$, while $|\boldsymbol{\varphi}_\gamma - \boldsymbol{\varphi}|$ is a small quantity of the order of $\varepsilon\boldsymbol{\varphi}$.

The definition of the internal bond tensors enables us to write the elasticity relations in explicit form. Actually, by substituting the expressions for the discrepancy vectors (9.2) into the elasticity relations (8.2), we obtain

$$\boldsymbol{\tau} = \boldsymbol{\tau}_0 + {}^4\mathbf{A} \cdot\cdot \boldsymbol{\varepsilon} + {}^4\mathbf{B} \cdot\cdot \boldsymbol{\kappa}, \quad \boldsymbol{\mu} = \boldsymbol{\mu}_0 + {}^4\tilde{\mathbf{B}} \cdot\cdot \boldsymbol{\varepsilon} + {}^4\mathbf{C} \cdot\cdot \boldsymbol{\kappa} \tag{9.5}$$

The macroscopic stiffness tensors ${}^4\mathbf{A}$, ${}^4\mathbf{B}$, ${}^4\tilde{\mathbf{B}}$, ${}^4\mathbf{C}$ are calculated using the formulae

$$\begin{aligned}
{}^4\mathbf{A} &= {}^4\mathbf{A}^* + \sum_{\beta,\gamma} ({}^3\mathbf{A}_\beta^\gamma \cdot [{}^3\mathbf{U}_\beta^\varepsilon - {}^3\mathbf{U}_\gamma^\varepsilon]^T + {}^4\mathbf{B}_\beta^\gamma \cdot [{}^3\boldsymbol{\Phi}_\beta^\varepsilon - {}^3\boldsymbol{\Phi}_\gamma^\varepsilon]^T) \\
{}^4\mathbf{B} &= {}^4\mathbf{B}^* + \sum_{\beta,\gamma} ({}^3\mathbf{A}_\beta^\gamma \cdot [{}^3\mathbf{U}_\beta^\kappa - {}^3\mathbf{U}_\gamma^\kappa]^T + {}^4\mathbf{B}_\beta^\gamma \cdot [{}^3\boldsymbol{\Phi}_\beta^\kappa - {}^3\boldsymbol{\Phi}_\gamma^\kappa]^T) \\
{}^4\tilde{\mathbf{B}} &= ({}^4\mathbf{B}^*)^T + \sum_{\beta,\gamma} (({}^3\mathbf{B}_\beta^\gamma)^t \cdot [{}^3\mathbf{U}_\beta^\varepsilon - {}^3\mathbf{U}_\gamma^\varepsilon]^T + {}^3\mathbf{C}_\beta^\gamma \cdot [{}^3\boldsymbol{\Phi}_\beta^\varepsilon - {}^3\boldsymbol{\Phi}_\gamma^\varepsilon]^T) \\
{}^4\mathbf{C} &= {}^4\mathbf{C}^* + \sum_{\beta,\gamma} (({}^3\mathbf{B}_\beta^\gamma)^t \cdot [{}^3\mathbf{U}_\beta^\kappa - {}^3\mathbf{U}_\gamma^\kappa]^T + {}^4\mathbf{C}_\beta^\gamma \cdot [{}^3\boldsymbol{\Phi}_\beta^\kappa - {}^3\boldsymbol{\Phi}_\gamma^\kappa]^T)
\end{aligned} \tag{9.6}$$

In the case of a third rank tensor, the operation of transposition is defined as follows:

$${}^3\mathbf{D} \Rightarrow D^{igk}\mathbf{e}_i\mathbf{e}_j\mathbf{e}_k \Rightarrow {}^3\mathbf{D}^T = D^{igk}\mathbf{e}_k\mathbf{e}_j\mathbf{e}_i \tag{9.7}$$

10. The energy approach to determining the strain tensors and discrepancy vectors

We will write the energy balance equation for two interacting particles, that is, particle γ in the initial cell and particle β in the cell α, in the form

$$\dot{W}_{\alpha\beta}^\gamma = \mathbf{F}_{\alpha\beta}^\gamma \cdot \dot{\boldsymbol{\varepsilon}}_{\alpha\beta}^\gamma + \mathbf{M}_{\alpha\beta}^\gamma \cdot \dot{\boldsymbol{\kappa}}_{\alpha\beta}^\gamma \tag{10.1}$$

Summing Eq. (10.1) over the indices α, β and γ, we obtain the energy balance equation for the whole system

$$\dot{W} = \sum_{\alpha,\beta,\gamma} \dot{W}_{\alpha\beta}^\gamma = \sum_{\alpha,\beta,\gamma} [\mathbf{F}_{\alpha\beta}^\gamma \cdot \dot{\boldsymbol{\varepsilon}}_{\alpha\beta}^\gamma + \mathbf{M}_{\alpha\beta}^\gamma \cdot \dot{\boldsymbol{\kappa}}_{\alpha\beta}^\gamma] \tag{10.2}$$

Using relations (7.2), which associate the strain vectors with the strain tensors (7.5) and the discrepancy vectors (7.4), we reduce Eq. (10.2) to the form

$$\begin{aligned}
\dot{W} &= \left(\sum_{\alpha,\beta,\gamma} \mathbf{F}_{\alpha\beta}^\gamma \mathbf{a}_\alpha\right) \cdot\cdot \dot{\boldsymbol{\varepsilon}} + \left(\sum_{\alpha,\beta,\gamma} \left[\mathbf{M}_{\alpha\beta}^\gamma - \frac{1}{2}\mathbf{a}_{\alpha\beta}^\gamma \times \mathbf{F}_{\alpha\beta}^\gamma\right]\mathbf{a}_\alpha\right) \cdot\cdot \dot{\boldsymbol{\kappa}} + \\
&+ \sum_{\beta,\gamma}\left[\left(\sum_\alpha \mathbf{F}_{\alpha\beta}^\gamma\right) \cdot \dot{\mathbf{u}}_\beta^\gamma + \left(\sum_\alpha \left[\mathbf{M}_{\alpha\beta}^\gamma - \frac{1}{2}\mathbf{a}_{\alpha\beta}^\gamma \times \mathbf{F}_{\alpha\beta}^\gamma\right] \cdot \dot{\boldsymbol{\varphi}}_\beta^\gamma\right)\right]
\end{aligned} \tag{10.3}$$

We now introduce the mass internal energy density into the treatment

$$\rho U = \frac{1}{2V_*} W = \frac{1}{2V_*} \sum_{\alpha,\beta,\gamma} W_{\alpha\beta}^\gamma \tag{10.4}$$

Then, using expressions (6.2) for the stress tensors $\boldsymbol{\tau}$ and $\boldsymbol{\mu}$ and expressions (6.6) for the stress vectors $\boldsymbol{\tau}_\beta^\gamma$ and $\boldsymbol{\mu}_\beta^\gamma$, Eq. (10.3) can be written in the form

$$(\rho U)^{\cdot} = \boldsymbol{\tau}^T \cdot\cdot\, \dot{\boldsymbol{\varepsilon}} + \boldsymbol{\mu}^T \cdot\cdot\, \dot{\boldsymbol{\kappa}} + \sum_{\beta,\gamma} [\boldsymbol{\tau}_\beta^\gamma \cdot \dot{\mathbf{u}}_\beta^\gamma + \boldsymbol{\mu}_\beta^\gamma \cdot \dot{\boldsymbol{\varphi}}_\beta^\gamma] \tag{10.5}$$

Hence, it has been proved that the quantities $\boldsymbol{\varepsilon}, \boldsymbol{\kappa}, \mathbf{u}_\beta^\gamma, \boldsymbol{\varphi}_\beta^\gamma$ introduced above are precisely those measures of the deformations for which the stress tensors $\boldsymbol{\tau}$ and $\boldsymbol{\mu}$ and the stress vectors $\boldsymbol{\tau}_\beta^\gamma$ and $\boldsymbol{\mu}_\beta^\gamma$ perform work. Note that strain tensors (7.5) are identical to the strain tensors in the macroscopic moment theory of elasticity. Then, according to the energy balance Eq. (10.5), the stress tensor $\boldsymbol{\tau}$ and the stress moment tensor $\boldsymbol{\mu}$, defined by formula (6.2), must be identical to the corresponding quantities in the macroscopic moment theory of elasticity.

11. The Cauchy–Green relations

We will now obtain the elastic relations using an energy approach. Since an elastic deformation of the system is considered, according to energy balance Eq. (10.5) the Cauchy–Green relations have the form

$$\boldsymbol{\tau} = \frac{\partial \rho U}{\partial \boldsymbol{\varepsilon}}, \quad \boldsymbol{\mu} = \frac{\partial \rho U}{\partial \boldsymbol{\kappa}}, \quad \boldsymbol{\tau}_\beta^\gamma = \frac{\partial pU}{\partial \mathbf{u}_\beta^\gamma}, \quad \boldsymbol{\mu}_\beta^\gamma = \frac{\partial \rho U}{\partial \boldsymbol{\varphi}_\beta^\gamma} \tag{11.1}$$

Hence, in order to obtain the relations between the stresses and strains using formulae (11.1), it is necessary to specify the internal energy density as a function of the strain tensors and the discrepancy vectors.

The energy of the interaction between a particle γ in the initial cell and a particle β in the cell α has the form

$$W_{\alpha\beta}^\gamma = \tilde{\mathbf{F}}_{\alpha\beta}^\gamma \cdot \boldsymbol{\varepsilon}_{\alpha\beta}^\gamma + \tilde{\mathbf{M}}_{\alpha\beta}^\gamma \cdot \boldsymbol{\kappa}_{\alpha\beta}^\gamma + \frac{1}{2}\boldsymbol{\varepsilon}_{\alpha\beta}^\gamma \cdot \tilde{\mathbf{A}}_{\alpha\beta}^\gamma \cdot \boldsymbol{\varepsilon}_{\alpha\beta}^\gamma + \boldsymbol{\varepsilon}_{\alpha\beta}^\gamma \cdot \tilde{\mathbf{B}}_{\alpha\beta}^\gamma \cdot \boldsymbol{\kappa}_{\alpha\beta}^\gamma + \frac{1}{2}\boldsymbol{\kappa}_{\alpha\beta}^\gamma \cdot \tilde{\mathbf{C}}_{\alpha\beta}^\gamma \cdot \boldsymbol{\kappa}_{\alpha\beta}^\gamma \tag{11.2}$$

On substituting the expression for the interaction of the two particles (11.2) and the expressions for the expressions for the strain vectors (7.2) into the formula for the mass density of the internal energy of system (10.4), we obtain an expression for the internal energy density in the form of a quadratic form of the strain tensors and the discrepancy vectors

$$\begin{aligned} \rho U = {} & \boldsymbol{\varepsilon}^T \cdot\cdot\, \boldsymbol{\tau}_0 + \boldsymbol{\kappa}^T \cdot\cdot\, \boldsymbol{\mu}_0 + \frac{1}{2}\boldsymbol{\varepsilon}^T \cdot\cdot\, {}^4\mathbf{A}^* \cdot\cdot\, \boldsymbol{\varepsilon} + \boldsymbol{\varepsilon}^T \cdot\cdot\, {}^4\mathbf{B}^* \cdot\cdot\, \boldsymbol{\kappa} + \frac{1}{2}\boldsymbol{\kappa}^T \cdot\cdot\, {}^4\mathbf{C}^* \cdot\cdot\, \boldsymbol{\kappa} + \\ & + \boldsymbol{\varepsilon}^T \cdot\cdot \sum_{\beta,\gamma} [{}^3\mathbf{A}_\beta^\gamma \cdot \mathbf{u}_\beta^\gamma + {}^3\mathbf{B}_\beta^\gamma \cdot \boldsymbol{\varphi}_\beta^\gamma] + \boldsymbol{\kappa}^T \cdot\cdot \sum_{\beta,\gamma} [({}^3\mathbf{B}_\beta^\gamma)^t \cdot \mathbf{u}_\beta^\gamma + {}^3\mathbf{C}_\beta^\gamma \cdot \boldsymbol{\varphi}_\beta^\gamma] + \\ & + \sum_{\beta,\gamma} \left[\tilde{\boldsymbol{\tau}}_\beta^\gamma \cdot \mathbf{u}_\beta^\gamma + \tilde{\boldsymbol{\mu}}_\beta^\gamma \cdot \boldsymbol{\varphi}_\beta^\gamma + \frac{1}{2}\mathbf{u}_\beta^\gamma \cdot \mathbf{A}_\beta^\gamma \cdot \mathbf{u}_\beta^\gamma + \mathbf{u}_\beta^\gamma \cdot \mathbf{B}_\beta^\gamma \cdot \boldsymbol{\varphi}_\beta^\gamma + \frac{1}{2}\boldsymbol{\varphi}_\beta^\gamma \cdot \mathbf{C}_\beta^\gamma \cdot \boldsymbol{\varphi}_\beta^\gamma \right] \end{aligned} \tag{11.3}$$

Substituting the expression for the internal energy density (11.3) into the Cauchy–Green relations (11.1), we obtain the elasticity relations in an implicit form, which are identical to relations (8.2). This confirms the logical consistency of the theory which has been constructed.

Substituting the expressions for the discrepancy vectors (9.2) into formula (11.3), after some reduction which take account of Eq. (8.6), we obtain an expression for the internal energy density in the form of a quadratic form of the strain tensors

$$\rho U = \boldsymbol{\varepsilon}^T \cdot\cdot\, \boldsymbol{\tau}_0 + \boldsymbol{\kappa}^T \cdot\cdot\, \boldsymbol{\mu}_0 + \frac{1}{2}(\boldsymbol{\varepsilon}^T \cdot\cdot\, {}^4\mathbf{A} \cdot\cdot\, \boldsymbol{\varepsilon} + \boldsymbol{\varepsilon}^T \cdot\cdot\, {}^4\mathbf{B} \cdot\cdot\, \boldsymbol{\kappa} + \boldsymbol{\kappa}^T \cdot\cdot\, {}^4\tilde{\mathbf{B}} \cdot\cdot\, \boldsymbol{\varepsilon} + \boldsymbol{\kappa} \cdot\cdot\, {}^4\mathbf{C} \cdot\cdot\, \boldsymbol{\kappa}) \tag{11.4}$$

The stiffness tensors and the initial stress tensors are defined by formulae (9.6).

Using formulae (9.4) and (9.6), it can be shown that the following identity holds

$$\boldsymbol{\varepsilon}^T \cdot\cdot\, {}^4\mathbf{B} \cdot\cdot\, \boldsymbol{\kappa} \equiv \boldsymbol{\kappa}^T \cdot\cdot\, {}^4\tilde{\mathbf{B}} \cdot\cdot\, \boldsymbol{\varepsilon} \tag{11.5}$$

Substituting the expression for the internal energy density (11.4) into the Cauchy–Green relations (11.1), we obtain elasticity relations in explicit form, that are identical to relations (9.5), which also confirms the logical consistency of the theory constructed. Note that the lattice strain tensors (7.5) are identical to the strain tensors in the macroscopic moment theory of elasticity. The elasticity relations (9.5) are also identical to the elasticity relations of the macroscopic theory. Then, the stress tensor $\boldsymbol{\tau}$ and the stress moment tensor $\boldsymbol{\mu}$, defined by formula (6.2), must be identical to the corresponding quantities in the macroscopic moment theory of elasticity.

12. Determination of the stiffness tensors of diatomic crystal lattices

We will now consider a complex crystal lattice, the unit cell of which contains two atoms: for example, a two-dimensional hexagonal lattice, the spatial lattice of graphite and diamond, the cubic lattice of NaCl, etc. In the case of such lattices, the system of equations for determining the stiffness tensor can be solved in explicit form. Below we will limit ourselves to cases when the equations for the force and moment stiffness tensors separate. However, it can be shown that an explicit solution also exists in the general case when there are cross stiffness tensors.

According to relations (9.4) and (9.6), when there are no cross stiffnesses the macroscopic stiffness tensors ${}^4\mathbf{A}$ and ${}^4\mathbf{C}$ are calculated using the formulae

$$ {}^4\mathbf{A} = {}^4\mathbf{A}^* + \sum_{\beta,\gamma} {}^3\mathbf{A}_\beta^\gamma \cdot [{}^3\mathbf{U}_\beta^\varepsilon - {}^3\mathbf{U}_\gamma^\varepsilon]^T, \quad {}^4\mathbf{C} = {}^4\mathbf{C}^* + \sum_{\beta,\gamma} {}^3\mathbf{C}_\beta^\gamma \cdot [{}^3\boldsymbol{\Phi}_\beta^\kappa - {}^3\boldsymbol{\Phi}_\gamma^\kappa]^T \tag{12.1} $$

where the intermediate variables, that is, the discrepancy tensors ${}^3\mathbf{U}_\gamma^\varepsilon$ and ${}^3\boldsymbol{\Phi}\gamma\kappa$, are determined by solving the two independent systems of M equations

$$ {}^3\mathbf{A}^\gamma + \sum_\beta [{}^3\mathbf{U}_\beta^\varepsilon - {}^3\mathbf{U}_\gamma^\varepsilon] \cdot \mathbf{A}_\beta^\gamma = 0, \quad {}^3\mathbf{C}^\gamma + \sum_\beta [{}^3\boldsymbol{\Phi}_\beta^\kappa - {}^3\boldsymbol{\Phi}_\gamma^\kappa] \cdot \mathbf{C}_\beta^\gamma = 0 \tag{12.2} $$

In the given case $M=2$ and the indices β and γ take the value 1 and 2. Moreover, identities (9.4) are satisfied in the case of the discrepancy tensors, that is,

$$ {}^3\mathbf{U}_1^\varepsilon + {}^3\mathbf{U}_2^\varepsilon = 0, \quad {}^3\boldsymbol{\Phi}_1^\kappa + {}^3\boldsymbol{\Phi}_2^\kappa = 0 \tag{12.3} $$

Consequently, of the four Eq. (12.2), only two are independent, for example, the equations when $\gamma=1$.

The simultaneous solution of Eq. (12.2) when $\gamma=1$ and Eq. (12.3) enables us to find the discrepancy tensors in explicit form

$$ {}^3\mathbf{U}_1^\varepsilon = \frac{1}{2}({}^3\mathbf{A}^1) \cdot (\mathbf{A}_2^1)^{-1}, \quad {}^3\boldsymbol{\Phi}_1^\kappa = \frac{1}{2}({}^3\mathbf{C}^1) \cdot (\mathbf{C}_2^1)^{-1} \tag{12.4} $$

and their substitution into formulae (12.1) enables us to obtain explicit expressions for the stiffness tensors

$$ {}^4\mathbf{A} = {}^4\mathbf{A}^* - 2({}^3\mathbf{A}_2^1) \cdot (\mathbf{A}_1^2)^{-T} \cdot ({}^3\mathbf{A}_2^1)^T, \quad {}^4\mathbf{C} = {}^4\mathbf{C}^* - 2({}^3\mathbf{C}_2^1) \cdot (\mathbf{C}_1^2)^{-T} \cdot ({}^3\mathbf{C}_2^1)^T \tag{12.5} $$

Here, we have used the notation $\mathbf{A}^{-T} \stackrel{\text{def}}{=} (A^{-1})^T$ and the identities

$$ {}^3\mathbf{A}^1 = {}^3\mathbf{A}_2^1 = -{}^3\mathbf{A}_1^2, \quad {}^3\mathbf{C}^1 = {}^3\mathbf{C}_2^1 = -{}^3\mathbf{C}_1^2 \tag{12.6} $$

13. Calculation of the stiffness tensors of a hexagonal lattice

The stiffness tensors for a hexagonal lattice (the two-dimensional lattice of graphite) are calculated in this section and the relation between the macroscopic moduli of elasticity and the stiffnesses of the interatomic bonds is determined.

13.1. The stiffnesses of the interatomic bonds

Since a two-dimensional lattice is considered, we shall assume that all of the atoms are located in a plane which is perpendicular to the unit vector $\mathbf{k}$ and that the rotations occur about the vector $\mathbf{k}$. We will represent the interatomic

bond stiffness tensors in the form

$$\mathbf{A}_{\alpha\beta}^{\gamma} = A_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma} + D_{\alpha\beta}^{\gamma}\mathbf{d}_{\alpha\beta}^{\gamma}\mathbf{d}_{\alpha\beta}^{\gamma}\mathbf{d}_{\alpha\beta}^{\gamma}, \quad \mathbf{C}_{\alpha\beta}^{\gamma} = C_{\alpha\beta}^{\gamma}\mathbf{k}\mathbf{k}; \quad \mathbf{d}_{\alpha\beta}^{\gamma} \stackrel{\text{def}}{=} \mathbf{k}\times\mathbf{a}_{\alpha\beta}^{\gamma} \tag{13.1}$$

According to the first formula of (13.1), the tensor $\mathbf{A}_{\alpha\beta}^{\gamma}$ does not contain a term proportional to the tensor $\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{d}_{\alpha\beta}^{\gamma} + \mathbf{d}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}$) (a cross term), which holds in the case of specific symmetries that exist in many crystal lattices, including a hexagonal lattice. The products $A_{\alpha\beta}^{\gamma}(a_{\alpha\beta}^{\gamma})^2$ and $D_{\alpha\beta}^{\gamma}(a_{\alpha\beta}^{\gamma})^2$ are the longitudinal and transverse stiffnesses of the interatomic bonds respectively. Note that the presence of transverse stiffnesses is evidence of the non-central character of the interatomic interaction. It is well known that a non-central interaction only occurs in moment theories.[15]

Substitution of expression (13.1) into relations (8.3) leads to the following expression for the stiffness tensors

$$^4\mathbf{A}^* = \frac{1}{2V_*}\sum_{\alpha,\beta,\gamma}(A_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma} + D_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{d}_{\alpha\beta}^{\gamma}\mathbf{d}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}), \; ^4\mathbf{C}^* = \frac{1}{2V_*}\sum_{\alpha,\beta,\gamma} C_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{k}\mathbf{k}\mathbf{a}_{\alpha\beta}^{\gamma}$$

$$^3\mathbf{A}_{\beta}^{\gamma} = \frac{1}{2V_*}\sum_{\alpha}(A_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma} + D_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{d}_{\alpha\beta}^{\gamma}\mathbf{d}_{\alpha\beta}^{\gamma}), \; ^3\mathbf{C}_{\beta}^{\gamma} = \frac{1}{2V_*}\sum_{\alpha} C_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{k}\mathbf{k} \tag{13.2}$$

$$\mathbf{A}_{\gamma}^{\beta} = \frac{1}{2V_*}\sum_{\alpha}(A_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma} + D_{\alpha\beta}^{\gamma}\mathbf{d}_{\alpha\beta}^{\gamma}\mathbf{d}_{\alpha\beta}^{\gamma}), \; \mathbf{C}_{\beta}^{\gamma} = \frac{1}{2V_*}\sum_{\alpha} C_{\alpha\beta}^{\gamma}\mathbf{k}\mathbf{k}$$

By virtue of the last formula of (13.1), the following identity holds

$$\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma} + \mathbf{d}_{\alpha\beta}^{\gamma}\mathbf{d}_{\alpha\beta}^{\gamma} = (\mathbf{a}_{\alpha\beta}^{\gamma})^2\mathbf{E} \tag{13.3}$$

where $\mathbf{E}$ is a two-dimensional unit vector. The identity (13.3) enables us to eliminate the vectors $\mathbf{d}_{\alpha\beta}^{\gamma}$ from formulae (13.2).

Note that the formulae obtained for the stiffness tensors hold for any number of atoms in a unit cell.

13.2. The use of the crystal lattice symmetry

The calculation of stiffness tensors is greatly simplified when use is made of spatial symmetry. A hexagonal lattice possesses third-order symmetry with respect to each lattice node (symmetry with respect to a rotation through an angle $2\pi/3$) and the intermediate stiffness tensors associated with the lattice nodes must possess the same symmetry. In the case of tensors of the first, second and fourth ranks, this leads to isotropy of the corresponding tensors. In the case of a first rank tensor (a vector), this means that the corresponding tensor must be zero and, in the case of a second-rank tensor, it must be spherical. Use of the above-mentioned considerations enables us to obtain the simplified formulae for the stiffness tensors (13.2)

$$^4\mathbf{A}^* = \frac{1}{2V_*}\sum_{\alpha,\beta,\gamma}\left[\left((A_{\alpha\beta}^{\gamma} - D_{\alpha\beta}^{\gamma})\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma} + \frac{1}{2}(D_{\alpha\beta}^{\gamma}(a_{\alpha\beta}^{\gamma})^4)\right)(\mathbf{iEi} + \mathbf{jEj})\right]$$

$$^4\mathbf{C}^* = \frac{1}{4V_*}\left(\sum_{\alpha,\beta,\gamma} C_{\alpha\beta}^{\gamma}(a_{\alpha\beta}^{\gamma})^2\right)(\mathbf{ikki} + \mathbf{jkkj}) \tag{13.4}$$

$$^3\mathbf{A}_{\beta}^{\gamma} = \frac{1}{2V_*}\sum_{\alpha}(A_{\alpha\beta}^{\gamma} - D_{\alpha\beta}^{\gamma})\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}\mathbf{a}_{\alpha\beta}^{\gamma}, \; ^3\mathbf{C}_{\beta}^{\gamma} = 0, \; \mathbf{A}_{\beta}^{\gamma} = \frac{1}{4V_*}\left(\sum_{\alpha}(A_{\alpha\beta}^{\gamma} + D_{\alpha\beta}^{\gamma})(a_{\alpha\beta}^{\gamma})^2\right)\mathbf{E}$$

where $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ are vectors forming an orthonormal basis. In deriving formulae (13.4), use has been made of identity $\mathbf{A} = (\mathrm{tr}\mathbf{A}/2)\mathbf{E}$ which is satisfied in the case of any spherical tensor and, also, identity (13.3). Taking account of the

formulae obtained, we will represent elasticity relations (12.5) in the form

$$^4\mathbf{A} = {}^4\mathbf{A}^* - \frac{4}{\mathrm{tr}\mathbf{A}_2^1}({}^3\mathbf{A}_2^1)\cdot({}^3\mathbf{A}_2^1)^T, \quad {}^4\mathbf{C} = {}^4\mathbf{C}^* \tag{13.5}$$

13.3. Determination of the components of the stiffness tensor

In the case of a hexagonal lattice, the resulting stiffness tensors $^4\mathbf{A}$ and $^4\mathbf{A}^*$ must possess sixth order symmetry, and this is only possible when they are isotropic. An arbitrary fourth-order isotropic tensor can be represented in the form of a linear combination of three tensors[16]

$$\mathbf{A} = A_1\mathbf{J}_1 + A_2\mathbf{J}_2 + A_3\mathbf{J}_3; \quad \mathbf{J}_1 \stackrel{\text{def}}{=} \mathbf{e}_k\mathbf{e}_k\mathbf{e}_n\mathbf{e}_n, \quad \mathbf{J}_2 \stackrel{\text{def}}{=} \mathbf{e}_k\mathbf{e}_n\mathbf{e}_n\mathbf{e}_k, \quad \mathbf{J}_3 \stackrel{\text{def}}{=} \mathbf{e}_k\mathbf{e}_n\mathbf{e}_k\mathbf{e}_n \tag{13.6}$$

where $\mathbf{e}_k$ are the vectors of a certain orthonormal basis. Summation over a repeated index is used in formula (13.6). In the two-dimensional case, the coefficients A_k can be calculated using the formulae

$$A_k = \frac{1}{8}\left(4A^k - \sum_{n=1}^{3} A^n\right), \quad A^k \stackrel{\text{def}}{=} \mathbf{A} \odot \mathbf{J}_k \tag{13.7}$$

where the symbol $\odot$ denotes tensor contraction: $\mathbf{A} \odot \mathbf{B} = A_{knpq}B_{qpnk}$. In other words, the quantities A^k are the contractions of the tensor $\mathbf{A}$ with respect to the corresponding pairs of vectors, for example,

$$A^1 = \sum_{k,n=1}^{3} A_{kknn} = \mathbf{E} \cdot\cdot \mathbf{A} \cdot\cdot \mathbf{E}$$

We will now calculate the tensor $^4\mathbf{A}$ (see formula (13.5)). We have

$$^4\mathbf{A} = {}^4\mathbf{A}^* - \frac{4}{\mathrm{tr}\mathbf{A}_2^1}{}^4\mathbf{Q}, \quad {}^4\mathbf{Q} \stackrel{\text{def}}{=} ({}^3\mathbf{A}_2^1)\cdot({}^3\mathbf{A}_2^1)^T \tag{13.8}$$

Calculation of the components of the expansion of the tensor $^4\mathbf{A}^*$ gives

$$A_1^* = A_3^* = \frac{1}{16V_*}\sum_{\alpha,\beta,\gamma}(A_{\alpha\beta}^\gamma - D_{\alpha\beta}^\gamma)(\mathbf{a}_{\alpha\beta}^\gamma)^4, \quad A_2^* = \frac{1}{16V_*}\sum_{\alpha,\beta,\gamma}(A_{\alpha\beta}^\gamma + 3D_{\alpha\beta}^\gamma)(\mathbf{a}_{\alpha\beta}^\gamma)^4 \tag{13.9}$$

The second term in the first formula of (13.8) is proportional to the fourth-rank tensor which is the product of two third-rank tensors. In the case of third-rank tensors, third-order symmetry does not lead to isotropy. However, their product, which is a fourth-rank tensor, must be isotropic which enables us to use expansion (13.6) and (13.7) in the case of the tensor $^4\mathbf{Q}$. It can be seen that $\mathbf{E}\cdot\cdot{}^3\mathbf{A}_2^1 \equiv 0$ (the product is a vector which, by virtue of the third-order symmetry, must be a zero vector) and, consequently, the following equality is satisfied

$$Q^1 = \mathbf{E} \cdot\cdot {}^4\mathbf{Q} \cdot\cdot \mathbf{E} = (\mathbf{E} \cdot\cdot {}^3\mathbf{A}_2^1)^2 = 0 \tag{13.10}$$

To calculate the remaining coefficients we make use of representation (13.4) for the tensor $^3\mathbf{A}_2^1$, which enables us to write the tensor $^4\mathbf{Q}$ in the form

$$^4\mathbf{Q} = \frac{1}{4V_{*\mu,\nu}^2}\sum(A_\mu - D_\mu)(A_\nu - D_\nu)\mathbf{a}_\mu\mathbf{a}_\mu\mathbf{a}_\mu\cdot\mathbf{a}_\nu\mathbf{a}_\nu\mathbf{a}_\nu \tag{13.11}$$

where the following notation is used

$$A_\mu = A_{\mu 2}^1, \quad D_\mu = D_{\mu 2}^1, \quad \mathbf{a}_\mu = \mathbf{a}_{\mu 2}^1$$

Then, using formula (13.7) for the components of the tensor ${}^4\mathbf{Q}$, we obtain

$$-Q_1 = Q_2 = Q_3 = \frac{1}{16V_*^2}\sum_{\mu,\nu}(A_\mu - D_\mu)(A_\nu - D_\nu)(\mathbf{a}_\mu \cdot \mathbf{a}_\nu)^3 \tag{13.12}$$

Substituting expressions (13.9) and (13.12) into elasticity relation (13.5), we conclude that the force interaction stiffness tensor ${}^4\mathbf{A}$ has the form

$$\mathbf{A} = A_1\mathbf{J}_1 + A_2\mathbf{J}_2 + A_3\mathbf{J}_3 \tag{13.13}$$

The coefficients A^k are defined by the formulae

$$\begin{aligned} A_{1,3} &= \frac{1}{16V_*}\left[\sum_{\alpha,\beta,\gamma}(A^\gamma_{\alpha\beta} - D^\gamma_{\alpha\beta})(\mathbf{a}^\gamma_{\alpha\beta})^4 \pm 8R\right] \\ A_2 &= \frac{1}{16V_*}\left[\sum_{\alpha,\beta,\gamma}(A^\gamma_{\alpha\beta} + 3D^\gamma_{\alpha\beta})(\mathbf{a}^\gamma_{\alpha\beta})^4 - 8R\right] \\ R &= \frac{\sum_{\mu,\nu}(A_\mu - D_\mu)(A_\nu - D_\nu)(\mathbf{a}_\mu \cdot \mathbf{a}_\nu)^3}{\sum_{\alpha}(A_\alpha + D_\alpha)(\mathbf{a}_\alpha)^2} \end{aligned} \tag{13.14}$$

In the two-dimensional case, the tensors $\mathbf{J}_k$ have the form

$$\begin{aligned} \mathbf{J}_1 &= \mathbf{e}_k\mathbf{e}_k\mathbf{e}_n\mathbf{e}_n = \mathbf{iiii} + \mathbf{jjjj} + \mathbf{iijj} + \mathbf{jjii} = \mathbf{EE} \\ \mathbf{J}_2 &= \mathbf{e}_k\mathbf{e}_n\mathbf{e}_n\mathbf{e}_k = \mathbf{iiii} + \mathbf{jjjj} + \mathbf{ijji} + \mathbf{jiij} = \mathbf{iEi} + \mathbf{jEj} \\ \mathbf{J}_3 &= \mathbf{e}_k\mathbf{e}_n\mathbf{e}_k\mathbf{e}_n = \mathbf{iiii} + \mathbf{jjjj} + \mathbf{ijij} + \mathbf{jiji} \end{aligned} \tag{13.15}$$

which enables us to express the projections of the tensor ${}^4\mathbf{A}$ in an orthonormal basis (the stiffness coefficients of an elastic medium) in terms of the coefficients A_k as follows:

$$\begin{aligned} &A_{1111} = A_{2222} = A_1 + A_2 + A_3, \quad A_{1122} = A_{2211} = A_1, \\ &A_{1221} = A_{2112} = A_2, \quad A_{1212} = A_{2121} = A_3 \end{aligned} \tag{13.16}$$

The coefficient of bulk compression K, corresponding to the tensor $\mathbf{A}$, can be determined in the two-dimensional case using one of the following formulae

$$4K = \mathbf{E}\cdot\cdot\mathbf{A}\cdot\cdot\mathbf{E} = A^1 = 2(2A_1 + A_2 + A_3) = A_{1111} + A_{2222} + A_{1122} + A_{2211} \tag{13.17}$$

which gives the value

$$K = \frac{1}{8V_*}\sum_{\alpha,\beta,\gamma}A^\gamma_{\alpha\beta}(\mathbf{a}^\gamma_{\alpha\beta})^4 \tag{13.18}$$

As would be expected, the coefficient of bulk compression depends solely on the coefficients $A^\gamma_{\alpha\beta}$ (which characterize the longitudinal stiffness of a bond) and is independent of the coefficients $D^\gamma_{\alpha\beta}$ (which characterize the transverse stiffness).

13.4. Interaction of the closest neighbours

We will now consider a hexagonal lattice with interaction of the nearest neighbours. Then, all of the non-zero stiffness coefficients of the interatomic bonds are equal to one another, which enables us to use the notation

$$A^\gamma_{\alpha\beta} = A_\alpha = A, \quad D^\gamma_{\alpha\beta} = D_\alpha = D, \quad C^\gamma_{\alpha\beta} = C \tag{13.19}$$

We will denote the distance between closest neighbours by a; then the volume of the unit cell is equal to

$$V_* = \frac{3\sqrt{3}}{2}a^2 \tag{13.20}$$

Each atom has three closest neighbours, and the unit cell contains two atoms Consequently, in formulae (13.14), the sums $\sum_{\alpha,\beta,\gamma}$ each contain six terms, and the sums $\sum_{\alpha}$ each contain three terms. Then,

$$\sum_{\mu,\nu}(\mathbf{a}_\mu \cdot \mathbf{a}_\nu)^3 = \frac{9}{4}a^6 \tag{13.21}$$

Substituting of expressions (13.19)–(13.21) into formulae (13.14) we obtain

$$A_1 = \frac{\sqrt{3}}{6}a^2 A\frac{A-D}{A+D}, \quad A_2 = \frac{\sqrt{3}}{6}a^2 D\frac{3A+D}{A+D}, \quad A_3 = \frac{\sqrt{3}}{6}a^2 D\frac{A-D}{A+D} \tag{13.22}$$

The coefficient of bulk compression, corresponding to the tensor $\mathbf{A}$, is equal to

$$K = \frac{1}{2}(2A_1 + A_2 + A_3) = \frac{\sqrt{3}}{6}a^2 A \tag{13.23}$$

For the moment stiffness tensor ${}^4\mathbf{C}$, with interaction of the nearest neighbours, from relations (13.4) and (13.5) we obtain

$${}^4\mathbf{C} = \sqrt{3}C(\mathbf{ikki} + \mathbf{jkkj}) \tag{13.24}$$

In the momentless case ($D = 0$), formulae (13.22) take the form

$$A_1 = \frac{\sqrt{3}}{6}a^2 A, \quad A_2 = A_3 = 0 \tag{13.25}$$

Hence, in the momentless case, the stiffness tensor of a hexagonal lattice in which only the nearest neighbours interact only has a spherical part:

$$\mathbf{A} = A_1\mathbf{EE} = K\mathbf{EE} \tag{13.26}$$

and, consequently, this lattice cannot resist a shear load.

13.5. Transition to the momentless theory of elasticity

Within the framework of the momentless theory of elasticity, the stress and strain tensors are symmetric, which enables us to determine the modulus A_1 and the sum of the moduli $A_2 + A_3$. No physical experiment, for which the results are processed within the framework of the momentless theory of elasticity, enables us to find the moduli A_2 and A_3 separately and since, the overwhelming majority of experiments are processed precisely in this way, the following moduli are of the greatest interest

$$A_1 = \frac{\sqrt{3}}{6}a^2 A\frac{A-D}{A+D}, \quad A_2 + A_3 = 2\frac{\sqrt{3}}{3}a^2\frac{AD}{A+D} \tag{13.27}$$

It is well known that only two independent elastic moduli exist in the momentless theory of elasticity, and the moduli (13.27) can be chosen as these moduli. If the values of the above-mentioned moduli are known for the material being considered, then, when the interatomic distance a is known, formulae (13.27) enable us to determine the microscopic characteristics of the interatomic bonds, that is, the coefficients A and D. Hence, the momentless macroscopic characteristics of a material enable us to determine not only the pure force characteristic of an interatomic bond A but, also, the coefficient D, which characterizes the transverse stiffness of an interatomic bond and exists only when there is an interaction moment at the atomic level.

We will now present formulae for the relation between the moduli (13.27) and the stiffness coefficients of an elastic medium

$$A_{1111} = A_{2222} = A_1 + A_2 + A_3, \quad A_{1122} = A_{2211} = A_1 \tag{13.28}$$

with shear modulus G, Young's modulus E and Poisson's ratio ν

$$G = A_{1212} = A_2 + A_3, \quad E = \frac{(A_1 + A_2 + A_3)^2 - A_1^2}{A_1 + A_2 + A_3}, \quad \nu = \frac{A_1}{A_1 + A_2 + A_3} \tag{13.29}$$

From formulae (13.27) and (13.28), it is easy to obtain formulae for the interatomic interaction coefficients

$$A = \frac{\sqrt{3}}{a^2}(A_{1111} + A_{1122}), \quad D = \frac{\sqrt{3}}{a^2}\frac{A_{1111}^2 - A_{1122}^2}{A_{1111} + 3A_{1122}} \tag{13.30}$$

As an example, we will consider the crystal lattice of graphite. In the case of this lattice[17,18]

$$A_{1111}/h = 1060 \text{ ГПа}, \quad A_{1122}/h = 180 \text{ ГПа}; \quad a = 0.142 \text{ нм}, \quad h = 0.34 \text{ нм} \tag{13.31}$$

where h is the distance between the graphite planes in graphite crystals. We recall that the coefficients (13.29)–(13.31) correspond to the two-dimensional theory, that is, they are measured in Nm^{-1} whereas the experimentally determined values of the stiffnesses of graphite correspond to the three-dimensional theory and, consequently, they are measured in $\text{Pa} = \text{Nm}^{-2}$. The distance h is the coefficient of proportionality between the two-dimensional and three-dimensional moduli of elasticity (since the volume of the three-dimensional unit cell of a graphite crystal is equal to the product of h and the area of a two-dimensional unit cell of a graphite layer).

From formulae (13.28), we obtain the values of the moduli of elasticity for graphite

$$A_1 = 61.2 \text{ Н/м}, \quad A_2 + A_3 = 299 \text{ Н/м} \tag{13.32}$$

and the values for the stiffnesses of the interatomic bonds in graphite crystals

$$Aa^2 = 730 \text{ Н/м}, \quad Da^2 = 402 \text{ Н/м} \tag{13.33}$$

follow from formulae (13.30).

Note that it is just the quantities Aa^2 and Da^2, rather than the coefficients A and D, that have a physical meaning and they are the stiffnesses of the interatomic bonds. According to the values (13.33) which have been obtained, the ratio of the transverse stiffness to the longitudinal stiffness for the bond between carbon atoms in graphite crystals is equal to

$$D/A = 0.55$$

Hence, the transverse stiffness of a covalent bond is comparable with the longitudinal stiffness and has to be taken into account in calculations involving covalent crystals.

14. Main results and conclusions

A discrete mechanical model of a complex crystal lattice has been proposed in which the atoms of the lattice are identified with particles of a general form, which possess both translational and rotational degrees of freedom and which interact with one another by means of forces and moments. Within the framework of linear theory, second-rank stiffness tensors, the structure of which is determined by the geometry of the lattice, are characteristics of the interatomic bonds, and the moduli of elasticity have to be found experimentally.

Using the long-wave approximation, the transition is made to a continual model of a complex crystal lattice. The equations describing the dynamics of the continual model are identical to the equations of the macroscopic moment theory of elasticity. The elastic properties of a lattice are characterized by fourth-rank macroscopic stiffness tensors. Expressions have been obtained for the macroscopic stiffness tensors, which depend on the stiffness tensors of the interatomic bonds and the vectors which determine the geometry of the lattice. Hence, if the microscopic characteristics

of the interatomic bonds are found from any kind of physical experiments, formulae (8.3), (8.5), (9.4) and (9.6) enable one to determine all the moduli of elasticity of the moment theory of elasticity.

A transition has been made to the momentless theory and it has been shown by taking the example of diatomic crystal lattices, that the macroscopic moduli of elasticity of the momentless theory depend both on the force characteristics as well as on the moment characteristics of the interatomic interaction. This dependence enables one to determine the microscopic characteristics of interatomic bonds, that is, the coefficients A and D. Hence, the moduli of elasticity of momentless macroscopic theory enable one to determine not only the purely force characteristic of an interatomic bond A but, also, the coefficient D, which characterizes the transverse stiffness of an interatomic bond and only exists when there is a moment interaction at the atomic level. In their turn, the coefficients A and D enable one to determine the parameters of the moment pair interaction potentials. The latter can be used as an alternative to multiparticle potentials in problems in the computer simulation of thermomechanical processes using methods of molecular dynamics.

The stiffnesses of the interatomic bonds in a layer of graphite have been calculated and it has been shown that the transverse stiffness of an interatomic bond is 55% of the longitudinal stiffness. This result shows that a covalent bond is substantially non-central, which is only possible when there are moment interactions at the atomic level.

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