

## DESCRIPTION OF CRYSTAL PACKING OF PARTICLES WITH TORQUE INTERACTION

E. A. Ivanova, A. M. Krivtsov, N. F. Morozov, and A. D. Firsova

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Pairwise interaction potentials, for example, Lennard–Jones, Mie, or Morse potentials, are widely utilized for modeling molecular systems. These potentials have a clear physical meaning and, although rather simple, enable one to describe the properties of a great number of substances on the qualitative level. It is well known, however, that these potentials have essential drawbacks that restrict their application area. One of the major drawbacks is that the pairwise potentials can provide stability only for crystal lattices with dense packing. This is a triangular lattice in the 2D case and a face-centered cubic lattice (or one similar to that) in the 3D case. 3D and 2D lattices with lower packing densities (e.g., a simple cubic lattice) are unstable for most of the pairwise potentials. This is for that reason that the distance between the second neighbors (along the diagonals of the cube) lies on the unstable segment of the force–distance diagram, i.e., an increase in this distance leads to a destabilizing, rather than restoring, force. This leads, for example, to the fact that the deformation of a square lattice into a rhombic one turns out to be energetically profitable. The structures characteristic of covalent crystals—hexagonal lattice on plane (graphite structure) and diamond structure in space—are also unstable. The traditional solution of this problem implies the utilization of many-body interaction potentials [1, 2]. These potentials depend on the angles between the bonds, which enables structures with low packing density to be stabilized. On the other hand, the expressions for these potentials are rather complex and constants occurring in these expressions do not have a clear physical meaning. These constants are adjusted so as to provide the best agreement of the calculated characteristics of substances to be modeled with those known from experiments. However, when proceeding from a crystal structure to another structure (for, example, from graphite to diamond), one has to completely change the interaction potential.

An alternative approach involves taking into account the torque component of the interatomic interaction. Covalent bonds are known to be directional, which enables these to transmit torque interactions. The necessity to take into account the torque interaction has been confirmed for polymers. An adequate description of the structural properties of polymer molecules is impossible without taking into account the torque interaction (corresponding to rotation about the bond direction). In the present paper, we will show that by taking into account pairwise torque interaction (in addition to the pairwise force interaction) one can provide the stability of crystal structures with low packing density. The torque interaction has a clear physical meaning and, for this reason, should be preferred to the many-body interaction.

However, the torque interaction is also rather complex in the general case. Therefore, a mechanical model of the torque interaction is needed which should, on the one hand, be fairly simple to admit a clear analytical formulation and, on the other hand, provide stability for crystal lattices under consideration. Such a model can be represented by groups of particles rigidly connected to one another and possessing a symmetry characteristic of the crystal structure. Each particle is a point mass interacting with particles of another group by means of pairwise force interaction. However, the total interaction between the groups will contain both the force and torque components. The resulting law of interaction can be applied to describe the interatomic interaction in a crystal with low packing density. This approach needs rather few parameters to be involved in the model. These are the parameters of the pairwise interaction and the geometrical parameters that characterize the groups of rigidly connected particles.

We anticipate that such an approach will enable one to construct models for most of the existing crystal structures and, moreover, will make it possible to describe the transition between the structures without changing the interaction law.

Equations of continuous theory of elasticity of media with rotational degrees of freedom are well known; see, e.g., [3]. In the present paper, we develop a model of a crystal packing of particles which yields the linear theory of couple stress elasticity in the long-wave approximation [4]. To that end, we apply the approach of [5, 6] that has been suggested for the couple-free case. The most difficult point in the description of the torque interaction between particles at the nodes of the crystal lattice is the definition of a strain measure and the derivation of constitutive relations. For the force interaction, the force acting between a pair of particles

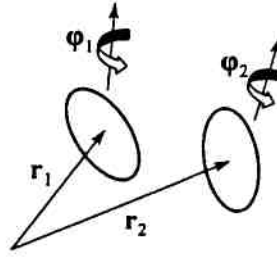


Fig. 1

is central, with the magnitude depending on the distance between the particles. The allowance for the torque interaction substantially complicates the situation. In this case, the force and torque vectors may have arbitrary directions, both of these vectors depending on the mutual position and mutual orientation of the particles. In what follows, to define the strain vector and to derive the constitutive relations for two interacting particles we utilize an approach similar to the technique employed in continuum mechanics to construct couple stress theories [7–10]. By means of this approach we show that the dynamics of the crystal lattice in the long-wave approximation is governed by the equations of macroscopic couple stress elasticity, irrespective of the structure of the particles. We obtain the expressions for the stiffness tensors of rank 4, which characterize the elastic properties of the crystal lattice, in terms of stiffness tensors of rank 2, which characterize the stiffness of the interatomic bonds, and vectors specifying the geometry of the lattice. To illustrate the proposed technique we investigate the stability of a square crystal lattice, with the torque interaction being taken into account. The torque interaction provides the stabilization of the crystal.

Consider two particles modeling atoms of a crystal lattice (Fig. 1). We will assume that the interaction between these particles is determined not only by their mutual position but also by their mutual orientation. This interaction is characterized by the force vector and the torque vector. To determine the force and torque as functions of the relative position and orientation of the particles, we will proceed exactly as is the case in the theory of shells and rods [7, 9]. In the actual configuration, the positions of the particles are defined by the position vectors,  $\mathbf{r}_1$  and  $\mathbf{r}_2$ , while the orientations are identified by the rotation vectors,  $\boldsymbol{\varphi}_1$  and  $\boldsymbol{\varphi}_2$ . At the equilibrium we have  $\mathbf{r}_2 - \mathbf{r}_1 = \mathbf{r}_0$ ,  $\boldsymbol{\varphi}_1 = \mathbf{0}$ , and  $\boldsymbol{\varphi}_2 = \mathbf{0}$ . Let  $\mathbf{F}_1$  and  $\mathbf{M}_1$  be the force and the torque, respectively, applied to particle 1 by particle 2,  $\mathbf{F}_2$  and  $\mathbf{M}_2$  the force and the torque applied to particle 2 by particle 1,  $\mathbf{F}_1^e$  and  $\mathbf{M}_1^e$  the external force and torque acting on particle 1, and  $\mathbf{F}_2^e$  and  $\mathbf{M}_2^e$  the external force and torque acting on particle 2. The torques  $\mathbf{M}_1$  and  $\mathbf{M}_1^e$  are defined with respect to particle 1, while the torques  $\mathbf{M}_2$  and  $\mathbf{M}_2^e$  with respect to particle 2. Following the theory of couple stress elasticity [11], we assume that the motion of individual particles 1 and 2 and the system of two particles is governed by the equations

$$\begin{aligned} m_1 \dot{\mathbf{v}}_1 &= \mathbf{F}_1 + \mathbf{F}_1^e, & (\boldsymbol{\theta}_1 \cdot \boldsymbol{\omega}_1)' &= \mathbf{M}_1 + \mathbf{M}_1^e, & m_2 \dot{\mathbf{v}}_2 &= \mathbf{F}_2 + \mathbf{F}_2^e, & (\boldsymbol{\theta}_2 \cdot \boldsymbol{\omega}_2)' &= \mathbf{M}_2 + \mathbf{M}_2^e, \\ (m_1 \mathbf{v}_1 + m_2 \mathbf{v}_2)' &= \mathbf{F}_1^e + \mathbf{F}_2^e, & (\mathbf{r}_1 \times m_1 \mathbf{v}_1 + \boldsymbol{\theta}_1 \cdot \boldsymbol{\omega}_1 + \mathbf{r}_2 \times m_2 \mathbf{v}_2 + \boldsymbol{\theta}_2 \cdot \boldsymbol{\omega}_2)' &= \mathbf{r}_1 \times \mathbf{F}_1^e + \mathbf{M}_1^e + \mathbf{r}_2 \times \mathbf{F}_2^e + \mathbf{M}_2^e, \end{aligned} \quad (1)$$

where  $m_1$  and  $m_2$  are the masses of particles 1 and 2,  $\boldsymbol{\theta}_1$  and  $\boldsymbol{\theta}_2$  are the tensors of inertia of these particles,  $\mathbf{v}_1$  and  $\mathbf{v}_2$  are the linear velocities, and  $\boldsymbol{\omega}_1$  and  $\boldsymbol{\omega}_2$  the angular velocities of the particles. Equations (1) imply Newton's third laws for forces and the analogue of this law for torques,

$$\mathbf{F}_1 + \mathbf{F}_2 = \mathbf{0}, \quad \mathbf{r}_1 \times \mathbf{F}_1 + \mathbf{M}_1 + \mathbf{r}_2 \times \mathbf{F}_2 + \mathbf{M}_2 = \mathbf{0}. \quad (2)$$

The balance of energy for the system of two particles is expressed by the relation

$$\left[ \frac{1}{2} (m_1 \mathbf{v}_1 \cdot \mathbf{v}_1 + \boldsymbol{\omega}_1 \cdot \boldsymbol{\theta}_1 \cdot \boldsymbol{\omega}_1 + m_2 \mathbf{v}_2 \cdot \mathbf{v}_2 + \boldsymbol{\omega}_2 \cdot \boldsymbol{\theta}_2 \cdot \boldsymbol{\omega}_2) + U \right]' = \mathbf{F}_1^e \cdot \mathbf{v}_1 + \mathbf{M}_1^e \cdot \boldsymbol{\omega}_1 + \mathbf{F}_2^e \cdot \mathbf{v}_2 + \mathbf{M}_2^e \cdot \boldsymbol{\omega}_2, \quad (3)$$

where  $U$  is the internal energy of the system (the interaction energy of particles 1 and 2). Assuming displacements from the equilibrium position to be small and taking into account Eqs. (1) and (2), one can reduce the equation of energy balance to the form

$$\begin{aligned} \dot{U} &= \mathbf{F} \cdot \dot{\boldsymbol{\varepsilon}} + \mathbf{M} \cdot \dot{\boldsymbol{\kappa}}, & \mathbf{F} &= \mathbf{F}_1 = -\mathbf{F}_2, & \boldsymbol{\varepsilon} &= \mathbf{r} - \mathbf{r}_0 + \frac{1}{2} \mathbf{r}_1 \times (\boldsymbol{\varphi}_1 + \boldsymbol{\varphi}_2), \\ \mathbf{M} &= \mathbf{M}_1 + \frac{1}{2} (\mathbf{r}_1 - \mathbf{r}_2) \times \mathbf{F}_1 = -\mathbf{M}_2 + \frac{1}{2} (\mathbf{r}_2 - \mathbf{r}_1) \times \mathbf{F}_2, & \boldsymbol{\kappa} &= \boldsymbol{\varphi}_2 - \boldsymbol{\varphi}_1, & \mathbf{r} &= \mathbf{r}_2 - \mathbf{r}_1. \end{aligned} \quad (4)$$

Here  $\mathbf{M}$  is the total torque exerted on particle 1 by particle 2 with respect to the midpoint of the segment connecting these particles. We will refer to the vectors  $\boldsymbol{\varepsilon}$  and  $\boldsymbol{\kappa}$ , on which the force and torque vectors perform work, as strain vectors. (See the relations of (4).) In what follows, we will consider elastic deformation of the system. We will assume that the internal energy, force, and torque depend only on the strain vectors but are independent on the strain rates. In this case we have

$$\mathbf{F} = \frac{\partial U}{\partial \boldsymbol{\varepsilon}}, \quad \mathbf{M} = \frac{\partial U}{\partial \boldsymbol{\kappa}}. \quad (5)$$

Since strains are assumed to be small, one can approximate the internal energy by the expression

$$U = \mathbf{F}^0 \cdot \boldsymbol{\varepsilon} + \mathbf{M}^0 \cdot \boldsymbol{\kappa} + \frac{1}{2} \boldsymbol{\varepsilon} \cdot \mathbf{A} \cdot \boldsymbol{\varepsilon} + \boldsymbol{\varepsilon} \cdot \mathbf{B} \cdot \boldsymbol{\kappa} + \frac{1}{2} \boldsymbol{\kappa} \cdot \mathbf{C} \cdot \boldsymbol{\kappa}. \quad (6)$$

The coefficients  $\mathbf{A}$ ,  $\mathbf{B}$ , and  $\mathbf{C}$  are called the stiffness tensors;  $\mathbf{F}^0$  and  $\mathbf{M}^0$  are called the initial force and initial torque, respectively. In the linear theory, the stiffness tensors are constant,  $\mathbf{A}$  and  $\mathbf{C}$  being symmetric tensors, while  $\mathbf{B}$  being arbitrary. In accordance with the relations of (5) and (6), the force and torque vectors have the form

$$\mathbf{F} = \mathbf{F}^0 + \mathbf{A} \cdot \boldsymbol{\varepsilon} + \mathbf{B} \cdot \boldsymbol{\kappa}, \quad \mathbf{M} = \mathbf{M}^0 + \boldsymbol{\varepsilon} \cdot \mathbf{B} + \mathbf{C} \cdot \boldsymbol{\kappa}. \quad (7)$$

On the basis of the theory of symmetry of tensors [7], one can show that if the internal structure of the particles is such that the system in the reference configuration is symmetric with respect to two mutually perpendicular planes, then the tensor  $\mathbf{B}$  vanishes. In this case, the expressions for the force and torques are simplified and have the form

$$\mathbf{F} = \mathbf{F}^0 + \mathbf{A} \cdot \boldsymbol{\varepsilon}, \quad \mathbf{M} = \mathbf{M}^0 + \mathbf{C} \cdot \boldsymbol{\kappa}. \quad (8)$$

This kind of symmetry is observed for most of simple crystal lattices. In what follows, when describing the crystal packing of particles within the framework of linear elasticity, we assume that  $\mathbf{B} = \mathbf{0}$  and that the interaction between the particles is characterized by the relations of (8).

*An alternative form for the relations of elasticity.* Previously, when deriving the relations of elasticity, we utilized the interaction torque  $\mathbf{M}$  calculated with respect to the midpoint of the segment connecting the interacting particles. In this case, the stiffness tensors  $\mathbf{B}$  and  $\mathbf{C}$  also should be interpreted as tensors about the midpoint of the segment connecting the particles. Such an approach is convenient for application of the theory of symmetry to identify the structure of the stiffness tensors. However, when deriving the equations of motion of a discrete medium it is more convenient to utilize the interaction torques calculated with respect to the particles. For this reason, in what follows, we will obtain the relations of elasticity in which the torque  $M_1$  applied by particle 2 to particle 1 is calculated with respect to particle 1. To that end, we rewrite Eq. (4) in the form

$$\dot{U} = \mathbf{F}_1 \cdot \dot{\boldsymbol{\varepsilon}}_1 + \mathbf{M}_1 \cdot \dot{\boldsymbol{\kappa}}_1, \quad \boldsymbol{\varepsilon}_1 = \mathbf{r} - \mathbf{r}_0 + \mathbf{r}_0 \times \boldsymbol{\varphi}_2, \quad \boldsymbol{\kappa}_1 = \boldsymbol{\varphi}_2 - \boldsymbol{\varphi}_1, \quad \mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1. \quad (9)$$

The vectors  $\boldsymbol{\varepsilon}_1$  and  $\boldsymbol{\kappa}_1$  on which the force vector,  $\mathbf{F}_1$ , and the torque vector,  $\mathbf{M}_1$ , perform work will be referred to as the strain vectors, as was the case for the vectors  $\boldsymbol{\varepsilon}$  and  $\boldsymbol{\kappa}$  of (4). In accordance to (9), the elasticity relations take the form

$$\mathbf{F}_1 = \frac{\partial U}{\partial \boldsymbol{\varepsilon}_1}, \quad \mathbf{M}_1 = \frac{\partial U}{\partial \boldsymbol{\kappa}_1}. \quad (10)$$

We assume the deformation to be small and express the internal energy as follows:

$$U = \tilde{\mathbf{F}}^0 \cdot \boldsymbol{\varepsilon}_1 + \tilde{\mathbf{M}}^0 \cdot \boldsymbol{\kappa}_1 + \frac{1}{2} \boldsymbol{\varepsilon}_1 \cdot \tilde{\mathbf{A}} \cdot \boldsymbol{\varepsilon}_1 + \boldsymbol{\varepsilon}_1 \cdot \tilde{\mathbf{B}} \cdot \boldsymbol{\kappa}_1 + \frac{1}{2} \boldsymbol{\kappa}_1 \cdot \tilde{\mathbf{C}} \cdot \boldsymbol{\kappa}_1. \quad (11)$$

Then, in accordance with (10) and (11), the force and torque vectors have the form

$$\mathbf{F}_1 = \tilde{\mathbf{F}}^0 + \tilde{\mathbf{A}} \cdot \boldsymbol{\varepsilon}_1 + \tilde{\mathbf{B}} \cdot \boldsymbol{\kappa}_1, \quad \mathbf{M}_1 = \tilde{\mathbf{M}}^0 + \boldsymbol{\varepsilon}_1 \cdot \tilde{\mathbf{B}} + \tilde{\mathbf{C}} \cdot \boldsymbol{\kappa}_1. \quad (12)$$

The stiffness tensors  $\tilde{\mathbf{A}}$ ,  $\tilde{\mathbf{B}}$ , and  $\tilde{\mathbf{C}}$  and the initial values of the force and torque vectors  $\tilde{\mathbf{F}}^0$  and  $\tilde{\mathbf{M}}^0$  differ from the stiffness tensors  $\mathbf{A}$ ,  $\mathbf{B}$ , and  $\mathbf{C}$  and the initial values of the force and torque vectors  $\mathbf{F}^0$  and  $\mathbf{M}^0$ . One can show that these quantities are related by

$$\tilde{\mathbf{F}}^0 = \mathbf{F}^0, \quad \tilde{\mathbf{M}}^0 = \mathbf{M}^0 + \frac{1}{2} \mathbf{r}_0 \times \mathbf{F}^0, \quad \tilde{\mathbf{A}} = \mathbf{A}, \quad \tilde{\mathbf{B}} = \mathbf{B} - \frac{1}{2} \mathbf{A} \times \mathbf{r}_0, \quad \tilde{\mathbf{C}} = \mathbf{C} - \frac{1}{4} \mathbf{B}^T \times \mathbf{r}^0 - \frac{1}{4} \mathbf{r}_0 \times \mathbf{A} \times \mathbf{r}_0. \quad (13)$$

When defining the concepts of the strain vectors for a system of two interacting particles we utilized an approach similar to that of continuum mechanics. We defined the strain vectors as vectors on which the force and torque vectors perform work. However, it is impossible to apply the relations of continuum mechanics straightforwardly to a discrete system. To clarify this statement, we will compare the continuum and discrete models. Since the system of two particles is a one-dimensional model, it should be compared with a rod. In the theory of rods, to define the force,  $\mathbf{F}$ , and the torque,  $\mathbf{M}$ , acting in a cross-section  $s$ , one mentally cuts the rod at this cross-section and removes one of the parts. The vectors  $\mathbf{F}$  and  $\mathbf{M}$  model the action of the removed part of the rod on the cross-section  $s$ , the torque  $\mathbf{M}$  being calculated with respect to this cross-section. In the discrete model, the interacting particles do not lie infinitely close to one another but are separated by the distance  $r_0$ . For that reason, it is impossible to introduce unambiguously the section  $s$ , with respect to which the torque  $\mathbf{M}$  should be calculated. Any point between 0 and  $r_0$  can play the role of this section. The value of the torque  $\mathbf{M}$  depends on the point with respect to which this torque is calculated, and hence, the value of the strain vector  $\varepsilon$  also depends on this point. (See the relations of (4) and (9).) The energy equation in the linear theory of rods can be reduced to the form

$$\rho \dot{U} = \mathbf{F} \cdot \dot{\varepsilon} + \mathbf{M} \cdot \dot{\boldsymbol{\kappa}}, \quad \varepsilon = \mathbf{u}' + \boldsymbol{\tau} \times \boldsymbol{\varphi}, \quad \boldsymbol{\kappa} = \boldsymbol{\varphi}', \quad (14)$$

where  $\rho U$  is the density of the internal energy,  $\mathbf{u}$  is the displacement vector of the section  $s$ ,  $\boldsymbol{\varphi}$  is the rotation vector of the section  $s$ ,  $\boldsymbol{\tau}$  is the unit vector tangent to the axis of the undeformed rod at the point  $s$ ,  $\varepsilon$  is the tensile strain vector, and  $\boldsymbol{\kappa}$  is the bending/torsion strain vector. Note that the strain vectors of the linear theory of rods (see (14)) characterize relative deformations, while the strain vectors of (4) and (9) introduced for the discrete system characterize absolute deformations. One can remove this mismatch by dividing the expressions for  $\varepsilon$  and  $\boldsymbol{\kappa}$  in the relations of (4) and (9) by  $r_0$ . As a result, the strain vectors in the discrete model of (4) and (9) and the strain vectors in the theory of rods (14) will have identical structures. However, an attempt to define the strain vectors  $\varepsilon$  and  $\boldsymbol{\kappa}$  for the discrete model by analogy with the relations of (14) leads to difficulties. When proceeding from the continuum model to the discrete model, one should replace the vector  $\mathbf{u}'$  by the difference  $\mathbf{r}_1 - \mathbf{r}_0$ , the vector  $\boldsymbol{\varphi}'$  by the difference  $\boldsymbol{\varphi}_2 - \boldsymbol{\varphi}_1$ , and the tangent unit vector  $\boldsymbol{\tau}$  by  $\mathbf{r}_0$ . However, it is impossible to define unambiguously an analogue of the vector of rotation of the rod's section,  $\boldsymbol{\varphi}$ , for the discrete system. The value of the vector  $\boldsymbol{\varphi}$  in the discrete system depends on the point with respect to which the torque of interaction between the particles is calculated. If the torque is calculated with respect to the middle point of the segment connecting the particles, then the analogue of the vector  $\boldsymbol{\varphi}$  in the discrete model is the half-sum of the rotation vectors of the particles. (See the relations of (4).) If the torque is calculated with respect to particle 1, then the analogue of the vector  $\boldsymbol{\varphi}$  in the discrete model is the rotation vector of particle 2. (See the relations of (9).) It should be noted that all these difficulties arise only in the couple stress theory. For purely force interaction, an analogy between the quantities characterizing the continuous and discrete models is obvious.

Consider a perfect simple crystal lattice. The lattice is formed by generic particles which interact with one another by forces and torques. (See the relations of (8).) We assume that each particle interacts with a bounded number of neighbors. Select a particle which, for convenience, will be referred to as the primary particle. We will number all particles which interact with the primary one. We will label the primary particle with the number  $\alpha = 0$  and the other particles with the numbers  $\alpha = \pm 1, \pm 2, \dots, \pm N$ . The particles are numbered so that the particles arranged symmetrically with respect to the primary particle have indices different in sign. Let  $\mathbf{a}_\alpha$  be the position vector of the particle number  $\alpha$  relative to the primary particle in the reference configuration. It is apparent that  $\mathbf{a}_{-\alpha} = -\mathbf{a}_\alpha$ . The position and orientation of the particle number  $\alpha$  are identified by the position vector,  $\mathbf{R}_\alpha$ , and the rotation vector,  $\boldsymbol{\varphi}_\alpha$ . In the reference configuration we have  $\mathbf{R}_\alpha = \mathbf{r}_\alpha$  and  $\boldsymbol{\varphi}_\alpha = \mathbf{0}$ . Let  $\mathbf{u}_\alpha$  denote the displacement of the particle number  $\alpha$ , i.e.,  $\mathbf{u}_\alpha = \mathbf{R}_\alpha - \mathbf{r}_\alpha$ . We will omit the index 0 in the notation of the position, displacement, and rotation vectors for the primary particle. We assume that the displacements and rotations are small and represent Euler's dynamic equations for the primary particle in the form

$$m \ddot{\mathbf{u}} = \sum_{\alpha} \mathbf{F}_\alpha + \mathbf{f}_*, \quad \boldsymbol{\theta} \cdot \ddot{\boldsymbol{\varphi}} = \sum_{\alpha} \mathbf{M}_\alpha + \mathbf{m}_*, \quad (15)$$

where  $m$  and  $\boldsymbol{\theta}$  are the mass and the tensor of inertia of the primary particle,  $\mathbf{F}_\alpha$  and  $\mathbf{M}_\alpha$  are the force and the torque exerted on the primary particle by the particle number  $\alpha$ , and  $\mathbf{f}_*$  and  $\mathbf{m}_*$  are the external force and torque. (The torques  $\mathbf{M}_\alpha$  and  $\mathbf{m}_*$  are calculated with respect to the primary particle.)

Consider two interacting particles—the primary particle with the position vector  $\mathbf{r}$  and the particle number  $-\alpha$  with the position vector  $\mathbf{r}_{-\alpha} = \mathbf{r} - \mathbf{a}_\alpha$ . The particle number  $-\alpha$  acts on the primary particle with the force  $\mathbf{F}_{-\alpha}(\mathbf{r})$  and the torque  $\mathbf{M}_{-\alpha}(\mathbf{r})$ , the torque being calculated with respect to the primary particle. The primary particle is the particle number  $\alpha$  with respect to the particle number  $-\alpha$ . Hence, the primary particle acts on the particle number  $-\alpha$  with the force  $\mathbf{F}_{-\alpha}(\mathbf{r} - \mathbf{a}_\alpha)$  and the torque  $\mathbf{M}_{-\alpha}(\mathbf{r} - \mathbf{a}_\alpha)$ , the torque being calculated with respect to the particle number  $-\alpha$ .

In accordance with Newton's third law for forces and the analogue of this law for torques (see the relations of (2)), we have

$$\mathbf{F}_{-\alpha}(\mathbf{r}) + \mathbf{F}_{\alpha}(\mathbf{r} - \mathbf{a}_{\alpha}) = \mathbf{0}, \quad \mathbf{M}_{-\alpha}(\mathbf{r}) + \frac{1}{2} \mathbf{a}_{\alpha} \times \mathbf{F}_{-\alpha}(\mathbf{r}) + \mathbf{M}_{\alpha}(\mathbf{r} - \mathbf{a}_{\alpha}) - \frac{1}{2} \mathbf{a}_{\alpha} \times \mathbf{F}_{\alpha}(\mathbf{r} - \mathbf{a}_{\alpha}) = \mathbf{0}. \quad (16)$$

Let  $\mathbf{F}_{\alpha}$  and  $\mathbf{M}_{\alpha}$  be defined not only for discrete  $\mathbf{r} \pm \mathbf{a}_{\alpha}$  but also for continuous  $\mathbf{r}$ , where  $\mathbf{r}$  is the position vector of an arbitrary point of the space. The specific definition of the functions  $\mathbf{F}_{\alpha}(\mathbf{r})$  and  $\mathbf{M}_{\alpha}(\mathbf{r})$  is unimportant. It is important, however, that these functions are differentiable and change little on the distances characteristic for interatomic interactions. Assuming the long-wave approximation [4] to be valid, we have

$$\mathbf{F}_{\alpha}(\mathbf{r} - \mathbf{a}_{\alpha}) \approx \mathbf{F}_{\alpha}(\mathbf{r}) - \mathbf{a}_{\alpha} \cdot \nabla \mathbf{F}_{\alpha}, \quad \mathbf{M}_{\alpha}(\mathbf{r} - \mathbf{a}_{\alpha}) \approx \mathbf{M}_{\alpha}(\mathbf{r}) - \mathbf{a}_{\alpha} \cdot \nabla \mathbf{M}_{\alpha}. \quad (17)$$

The relations of (16) and (17) imply

$$\mathbf{F}_{-\alpha}(\mathbf{r}) \approx -\mathbf{F}_{\alpha}(\mathbf{r}) + \nabla \cdot \mathbf{a}_{\alpha} \mathbf{F}_{\alpha}, \quad \mathbf{M}_{-\alpha}(\mathbf{r}) \approx -\mathbf{M}_{\alpha}(\mathbf{r}) + \mathbf{a}_{\alpha} \times \mathbf{F}_{\alpha}(\mathbf{r}) + \nabla \cdot \mathbf{a}_{\alpha} (\mathbf{M}_{\alpha} - \mathbf{a}_{\alpha} \times \mathbf{F}_{\alpha}). \quad (18)$$

Using the relations of (18), we obtain

$$\begin{aligned} \sum_{\alpha} \mathbf{F}_{\alpha} &= \sum_{\alpha} \mathbf{F}_{-\alpha} = \frac{1}{2} \sum_{\alpha} (\mathbf{F}_{\alpha} + \mathbf{F}_{-\alpha}) = \nabla \cdot \frac{1}{2} \sum_{\alpha} \mathbf{a}_{\alpha} \mathbf{F}_{\alpha}, \\ \sum_{\alpha} \mathbf{M}_{\alpha} &= \sum_{\alpha} \mathbf{M}_{-\alpha} = \frac{1}{2} \sum_{\alpha} (\mathbf{M}_{\alpha} + \mathbf{M}_{-\alpha}) = \left( \frac{1}{2} \sum_{\alpha} \mathbf{a}_{\alpha} \mathbf{F}_{\alpha} \right)_{\times} + \nabla \cdot \frac{1}{2} \sum_{\alpha} \mathbf{a}_{\alpha} (\mathbf{M}_{\alpha} - \mathbf{a}_{\alpha} \times \mathbf{F}_{\alpha}). \end{aligned} \quad (19)$$

Note that  $\mathbf{M}_{\alpha} - \mathbf{a}_{\alpha} \times \mathbf{F}_{\alpha}$  is the torque exerted on the primary particle by the particle number  $\alpha$  about the particle number  $\alpha$ . Denote

$$\boldsymbol{\tau} = \frac{1}{2V_*} \sum_{\alpha} \mathbf{a}_{\alpha} \mathbf{F}_{\alpha}, \quad \boldsymbol{\mu} = \frac{1}{2V_*} \sum_{\alpha} (\mathbf{M}_{\alpha} - \mathbf{a}_{\alpha} \times \mathbf{F}_{\alpha}), \quad (20)$$

where  $V_*$  is the volume of the elementary cell. The tensors  $\boldsymbol{\tau}$  and  $\boldsymbol{\mu}$  will be referred to as the stress tensor and the couple stress tensor, respectively. Denote

$$\rho = \frac{m}{V_*}, \quad \rho \boldsymbol{\vartheta} = \frac{1}{V_*} \boldsymbol{\theta}, \quad \mathbf{f} = \frac{1}{V_*} \mathbf{f}_*, \quad \mathbf{m} = \frac{1}{V_*} \mathbf{m}_*, \quad (21)$$

where  $\rho$  is the mass density of the medium,  $\boldsymbol{\vartheta}$  is the tensor of inertia of the medium per unit mass (mass density of the tensor of inertia),  $\mathbf{f}$  is the volume density of the external forces, and  $\mathbf{m}$  is the volume density of the external torques. With reference to the relations of (19)–(21), we rewrite the equations of (15), which govern the motion of the particle under consideration, as follows:

$$\nabla \cdot \boldsymbol{\tau} + \mathbf{f} = \rho \ddot{\mathbf{u}}, \quad \nabla \cdot \boldsymbol{\mu} + \boldsymbol{\tau}_{\times} + \mathbf{m} = \rho \boldsymbol{\vartheta} \cdot \ddot{\boldsymbol{\varphi}}. \quad (22)$$

The structure of equations (22) coincides with that of the dynamic equations of macroscopic couple stress elasticity.

In accordance with (20), the couple stress tensor can be expressed in terms of the torques  $\mathbf{M}_{\alpha}$  calculated with respect to the primary particle. For this reason, in what follows, we utilize the elasticity relations in the form of (12),

$$\mathbf{F}_{\alpha} = \tilde{\mathbf{F}}_{\alpha}^0 + \tilde{\mathbf{A}}_{\alpha} \cdot \boldsymbol{\varepsilon}_{\alpha} + \tilde{\mathbf{B}}_{\alpha} \cdot \boldsymbol{\kappa}_{\alpha}, \quad \mathbf{M}_{\alpha} = \tilde{\mathbf{M}}_{\alpha}^0 + \boldsymbol{\varepsilon}_{\alpha} \cdot \tilde{\mathbf{B}}_{\alpha} + \tilde{\mathbf{C}}_{\alpha} \cdot \boldsymbol{\kappa}_{\alpha}, \quad (23)$$

where the strain vectors  $\boldsymbol{\varepsilon}_{\alpha}$   $\boldsymbol{\kappa}_{\alpha}$  are defined by the relations of (9) and have the form

$$\boldsymbol{\varepsilon}_{\alpha} = \mathbf{u}_{\alpha} - \mathbf{u} + \mathbf{a}_{\alpha} \times \boldsymbol{\varphi}_{\alpha}, \quad \boldsymbol{\kappa}_{\alpha} = \boldsymbol{\varphi}_{\alpha} - \boldsymbol{\varphi}. \quad (24)$$

Utilizing the long-wave approximation [4], we write

$$\mathbf{u}_{\alpha} = \mathbf{u}(\mathbf{r} + \mathbf{a}_{\alpha}) \approx \mathbf{u}(\mathbf{r}) + \mathbf{a}_{\alpha} \cdot \nabla \mathbf{u}, \quad \boldsymbol{\varphi}_{\alpha} = \boldsymbol{\varphi}(\mathbf{r} + \mathbf{a}_{\alpha}) \approx \boldsymbol{\varphi}(\mathbf{r}) + \mathbf{a}_{\alpha} \cdot \nabla \boldsymbol{\varphi}. \quad (25)$$

Then the expressions of (24) for the strain vectors become

$$\boldsymbol{\varepsilon}_{\alpha} = \mathbf{a}_{\alpha} \cdot \nabla \mathbf{u} + \mathbf{a}_{\alpha} \times (\boldsymbol{\varphi} + \mathbf{a}_{\alpha} \cdot \nabla \boldsymbol{\varphi}), \quad \boldsymbol{\kappa}_{\alpha} = \mathbf{a}_{\alpha} \cdot \nabla \boldsymbol{\varphi}. \quad (26)$$

In what follows, we assume  $\mathbf{B}_\alpha = \mathbf{0}$ ; then  $\tilde{\mathbf{B}}_\alpha = -\frac{1}{2}\mathbf{A}_\alpha \times \mathbf{a}_\alpha$ . Substitute the expressions of (26) into the elasticity relations of (23) and make use of the relationships of (13) between the stiffness tensors to obtain (after simple transformations)

$$\begin{aligned} \mathbf{F}_\alpha &= \mathbf{F}_\alpha^0 + \mathbf{A}_\alpha \mathbf{a}_\alpha \cdot (\nabla \mathbf{u} + \mathbf{E} \times \boldsymbol{\varphi}) + \frac{1}{2} \mathbf{A}_\alpha \times \mathbf{a}_\alpha \mathbf{a}_\alpha \cdot \boldsymbol{\varphi}, \\ \mathbf{M}_\alpha &= \mathbf{M}_\alpha^0 + \frac{1}{2} \mathbf{a}_\alpha \times \mathbf{F}_\alpha^0 + \frac{1}{2} \mathbf{a}_\alpha \times \mathbf{A}_\alpha \mathbf{a}_\alpha \cdot (\nabla \mathbf{u} + \mathbf{E} \times \boldsymbol{\varphi}) + \left( \frac{1}{2} \mathbf{a}_\alpha \times \mathbf{A}_\alpha \times \mathbf{a}_\alpha + \tilde{\mathbf{C}}_\alpha \right) \mathbf{a}_\alpha \cdot \nabla \boldsymbol{\varphi}, \end{aligned} \quad (27)$$

where  $\mathbf{E}$  is the identity tensor. Denote

$$\boldsymbol{\varepsilon} = \nabla \mathbf{u} + \mathbf{E} \times \boldsymbol{\varphi}, \quad \boldsymbol{\kappa} = \nabla \boldsymbol{\varphi}. \quad (28)$$

We will refer to the tensors  $\boldsymbol{\varepsilon}$  and  $\boldsymbol{\kappa}$  as strain tensors. Note that the tensors of (28) coincide with the strain tensors of the macroscopic couple stress elasticity. By substituting the expressions of (27) and (28) into the expressions of (20) for the stress tensor and couple stress tensor we obtain

$$\boldsymbol{\tau} = \boldsymbol{\tau}_0 + {}^4\mathbf{A} \cdot \boldsymbol{\varepsilon} + {}^4\mathbf{B}_1 \cdot \boldsymbol{\kappa}, \quad \boldsymbol{\mu} = \boldsymbol{\mu}_0 + {}^4\mathbf{B}_2 \cdot \boldsymbol{\varepsilon} + {}^4\mathbf{C} \cdot \boldsymbol{\kappa}, \quad (29)$$

where the initial stress tensors,  $\boldsymbol{\tau}_0$  and  $\boldsymbol{\mu}_0$ , and the stiffness tensors,  ${}^4\mathbf{A}$ ,  ${}^4\mathbf{B}_1$ ,  ${}^4\mathbf{B}_2$ , and  ${}^4\mathbf{C}$ , are defined by

$$\begin{aligned} \boldsymbol{\tau}_0 &= \frac{1}{2V_*} \sum_\alpha \mathbf{a}_\alpha \mathbf{F}_\alpha^0, \quad \boldsymbol{\mu}_0 = \frac{1}{2V_*} \sum_\alpha \mathbf{a}_\alpha \left( \mathbf{M}_\alpha^0 - \frac{1}{2} \mathbf{a}_\alpha \times \mathbf{F}_\alpha^0 \right), \quad {}^4\mathbf{A} = \frac{1}{2V_*} \sum_\alpha \mathbf{a}_\alpha \mathbf{A}_\alpha \mathbf{a}_\alpha, \\ {}^4\mathbf{B}_1 &= \frac{1}{4V_*} \sum_\alpha \mathbf{a}_\alpha \mathbf{A}_\alpha \times \mathbf{a}_\alpha \mathbf{a}_\alpha, \quad {}^4\mathbf{B}_2 = -\frac{1}{4V_*} \sum_\alpha \mathbf{a}_\alpha \mathbf{a}_\alpha \times \mathbf{A}_\alpha \mathbf{a}_\alpha, \quad {}^4\mathbf{C} = \frac{1}{2V_*} \sum_\alpha \mathbf{a}_\alpha \tilde{\mathbf{C}}_\alpha \mathbf{a}_\alpha. \end{aligned} \quad (30)$$

Equations (22), (28), and (30) form a complete system of equations governing the motion of the atoms of a simple crystal lattice. The stiffness tensors and the initial stress tensors occurring in these equations can be expressed in terms of quantities characterizing the stiffness of the interatomic interactions and the structure of the crystal lattice in accordance with (30).

Consider the energy equation for two interacting particles—the primary particle and the particle number  $\alpha$ —represented in the form of (9),

$$\dot{W}_\alpha = \mathbf{F}_\alpha \cdot \dot{\boldsymbol{\varepsilon}}_\alpha + \mathbf{M}_\alpha \cdot \dot{\boldsymbol{\kappa}}_\alpha. \quad (31)$$

By summing the equations of (31) with respect to  $\alpha$  we obtain the energy equation for the entire system,

$$\dot{W} = \sum_\alpha \dot{W}_\alpha = \sum_\alpha (\mathbf{F}_\alpha \cdot \dot{\boldsymbol{\varepsilon}}_\alpha + \mathbf{M}_\alpha \cdot \dot{\boldsymbol{\kappa}}_\alpha). \quad (32)$$

Using the expressions of (26) and (28) for strain vectors and tensors, one can readily show that Eq. (32) can be reduced to the form

$$\dot{W} = \left( \sum_\alpha \mathbf{F}_\alpha \mathbf{a}_\alpha \right) \cdot \dot{\boldsymbol{\varepsilon}} + \left[ \sum_\alpha (\mathbf{M}_\alpha - \mathbf{a}_\alpha \times \mathbf{F}_\alpha) \mathbf{a}_\alpha \right] \cdot \dot{\boldsymbol{\kappa}}. \quad (33)$$

Introduce the mass density of the internal energy

$$\rho U = \frac{1}{2V_*} W. \quad (34)$$

Then, with reference to the expressions of (20) for the stress tensor  $\boldsymbol{\tau}$  and the couple stress tensor  $\boldsymbol{\mu}$ , one can represent Eq. (33) in the form

$$(\rho U) \cdot = \boldsymbol{\tau}^T \cdot \dot{\boldsymbol{\varepsilon}} + \boldsymbol{\mu}^T \cdot \dot{\boldsymbol{\kappa}}. \quad (35)$$

Thus we have proved that the quantities  $\boldsymbol{\varepsilon}$  and  $\boldsymbol{\kappa}$  are just the strain tensors on which the stress tensor,  $\boldsymbol{\tau}$ , and the couple stress tensor,  $\boldsymbol{\mu}$ , perform work. Note that the strain tensors of (28) completely coincide with the strain tensors of macroscopic couple stress elasticity. Then, in accordance with the energy equation of (35), the stress tensor  $\boldsymbol{\tau}$  and the couple stress tensor  $\boldsymbol{\mu}$  must completely coincide with the corresponding quantities of macroscopic couple stress elasticity. Since we consider elastic deformation of the system, the energy equation of (35) implies the elasticity relations in the form

$$\boldsymbol{\tau}^T = \frac{\partial(\rho U)}{\partial \boldsymbol{\varepsilon}}, \quad \boldsymbol{\mu}^T = \frac{\partial(\rho U)}{\partial \boldsymbol{\kappa}}. \quad (36)$$

Represent the density of the internal energy in the form

$$\rho U = \tau_0^T \cdot \varepsilon + \mu_0^T \cdot \boldsymbol{\chi} + \frac{1}{2} \varepsilon \cdot \cdot {}^4\mathbf{A}_* \cdot \varepsilon + \varepsilon \cdot \cdot {}^4\mathbf{B}_* \cdot \boldsymbol{\chi} + \frac{1}{2} \boldsymbol{\chi} \cdot \cdot {}^4\mathbf{C}_* \cdot \boldsymbol{\chi}, \quad (37)$$

where  ${}^4\mathbf{A}_*$ ,  ${}^4\mathbf{B}_*$ , and  ${}^4\mathbf{C}_*$  are coefficients having the sense of stiffness tensors, and then substitute the resulting expressions into the elasticity relations of (36) to obtain

$$\boldsymbol{\tau}^T = \tau_0^T + {}^4\mathbf{A}_* \cdot \varepsilon + {}^4\mathbf{B}_* \cdot \boldsymbol{\chi}, \quad \boldsymbol{\mu}^T = \mu_0^T + \varepsilon \cdot \cdot {}^4\mathbf{B}_* + {}^4\mathbf{C}_* \cdot \boldsymbol{\chi}. \quad (38)$$

By comparing the expressions of (38) with those of (29) one can readily establish the relationship between the stiffness tensors  ${}^4\mathbf{A}_*$ ,  ${}^4\mathbf{B}_*$ ,  ${}^4\mathbf{C}_*$  and  ${}^4\mathbf{A}$ ,  ${}^4\mathbf{B}_1$ ,  ${}^4\mathbf{B}_2$ ,  ${}^4\mathbf{C}$ . Make use of the theorem on the spectral expansion of a symmetric tensor to represent the tensors  $\mathbf{A}_\alpha$  and  $\tilde{\mathbf{C}}_\alpha$  of rank 2 by series in terms of the eigenvectors,

$$\mathbf{A}_\alpha = \sum_{n=1}^3 A_{\alpha n} \mathbf{e}_n \mathbf{e}_n, \quad \tilde{\mathbf{C}}_\alpha = \sum_{n=1}^3 \tilde{C}_{\alpha n} \mathbf{e}_n \mathbf{e}_n. \quad (39)$$

Then the stiffness tensors (30) of the crystal lattice, occurring as coefficients in the expressions of (29) for  $\boldsymbol{\tau}$  and  $\boldsymbol{\mu}$ , take the form

$$\begin{aligned} {}^4\mathbf{A} &= \frac{1}{2V_*} \sum_{\alpha} \sum_{n=1}^3 A_{\alpha n} \mathbf{a}_\alpha \mathbf{e}_n \mathbf{e}_n \mathbf{a}_\alpha, & {}^4\mathbf{B}_1 &= \frac{1}{4V_*} \sum_{\alpha} \sum_{n=1}^3 A_{\alpha n} \mathbf{a}_\alpha \mathbf{e}_n \mathbf{e}_n \times \mathbf{a}_\alpha \mathbf{a}_\alpha, \\ {}^4\mathbf{B}_2 &= \frac{1}{4V_*} \sum_{\alpha} \sum_{n=1}^3 A_{\alpha n} \mathbf{a}_\alpha \mathbf{e}_n \times \mathbf{a}_\alpha \mathbf{e}_n \mathbf{a}_\alpha, & {}^4\mathbf{C} &= \frac{1}{2V_*} \sum_{\alpha} \sum_{n=1}^3 \tilde{C}_{\alpha n} \mathbf{a}_\alpha \mathbf{e}_n \mathbf{e}_n \mathbf{a}_\alpha. \end{aligned} \quad (40)$$

The stiffness tensors  ${}^4\mathbf{A}_*$ ,  ${}^4\mathbf{B}_*$ , and  ${}^4\mathbf{C}_*$ , occurring as coefficients in the expressions of (38) for  $\boldsymbol{\tau}^T$  and  $\boldsymbol{\mu}^T$ , take the form

$$\begin{aligned} {}^4\mathbf{A}_* &= \frac{1}{2V_*} \sum_{\alpha} \sum_{n=1}^3 A_{\alpha n} \mathbf{e}_n \mathbf{a}_\alpha \mathbf{e}_n \mathbf{a}_\alpha, & {}^4\mathbf{C}_* &= \frac{1}{2V_*} \sum_{\alpha} \sum_{n=1}^3 \tilde{C}_{\alpha n} \mathbf{e}_n \mathbf{a}_\alpha \mathbf{e}_n \mathbf{a}_\alpha, \\ {}^4\mathbf{B}_* &= \frac{1}{4V_*} \sum_{\alpha} \sum_{n=1}^3 A_{\alpha n} \mathbf{e}_n \mathbf{a}_\alpha \mathbf{e}_n \times \mathbf{a}_\alpha \mathbf{a}_\alpha. \end{aligned} \quad (41)$$

It is apparent that the tensors of (41) can be obtained from the tensors of (40) by permuting the indices in the quadruples.

Consider as an example a particle formed by an arbitrary set of point masses rigidly connected to one another. The interaction of point masses belonging to different particles is characterized by the potential  $\Pi(r)$ . Consider the interaction of two identical particles. Let  $\mathbf{r}_1$  and  $\mathbf{r}_2$  be the position vectors of the centers of mass of these particles and  $\boldsymbol{\xi}_k$  the absolute position vectors of point masses belonging to these particles. Let the index  $k$  change from 1 to  $N$  for the first particle and from  $N+1$  to  $2N$  for the second particle. Then the force applied by particle 2 to particle 1 can be represented in the form

$$\mathbf{F} = \sum_{k=1}^N \sum_{n=N+1}^{2N} \mathbf{f}(\boldsymbol{\xi}_{kn}), \quad \boldsymbol{\xi}_{kn} \stackrel{\text{def}}{=} \boldsymbol{\xi}_k - \boldsymbol{\xi}_n, \quad \mathbf{f}(\boldsymbol{\xi}) \stackrel{\text{def}}{=} -\frac{d}{d\xi} \Pi(\xi), \quad \xi = |\boldsymbol{\xi}|. \quad (42)$$

The torque exerted on particle 1 by particle 2, calculated with respect to the center of the segment connecting these particles, is defined by

$$\mathbf{M} = \sum_{k=1}^N \sum_{n=N+1}^{2N} (\boldsymbol{\xi}_k - \mathbf{r}_c) \times \mathbf{f}(\boldsymbol{\xi}_{kn}), \quad \mathbf{r}_c \stackrel{\text{def}}{=} \frac{1}{2}(\mathbf{r}_1^0 + \mathbf{r}_2^0), \quad (43)$$

where  $\mathbf{r}_1^0$  and  $\mathbf{r}_2^0$  are the values of  $\mathbf{r}_1$  and  $\mathbf{r}_2$  in the equilibrium position. The force of interaction between the point masses forming the particles can be expressed by

$$\mathbf{f}(\boldsymbol{\xi}) = \Phi(\xi^2) \boldsymbol{\xi}, \quad \Phi(\xi^2) \stackrel{\text{def}}{=} -\frac{1}{\xi} \Pi'(\xi). \quad (44)$$

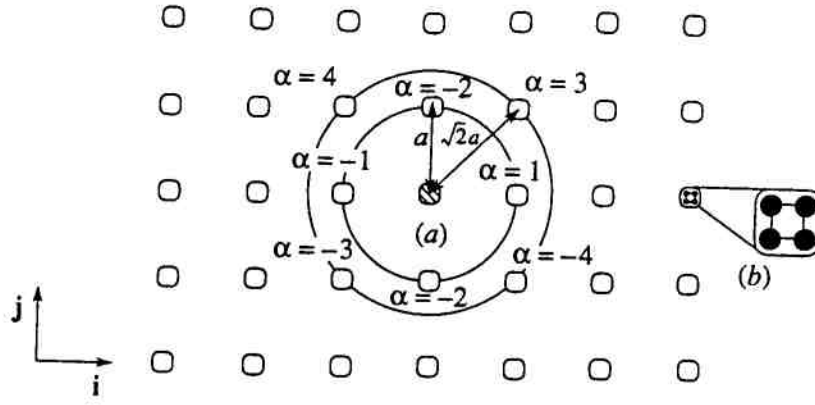


Fig. 2

With reference to (44), the relations of (42) and (43) become

$$\mathbf{F} = \sum_{k,n} \Phi(\xi_{kn}^2) \xi_{kn}, \quad \mathbf{M} = \sum_{k,n} (\xi_k - \mathbf{r}_c) \times \Phi(\xi_{kn}^2) \xi_{kn}. \quad (45)$$

Here and in what follows we omit the limits of the summation and assume that  $k$  changes from 1 to  $N$  and  $n$  from  $N+1$  to  $2N$ .

Consider small motions of the system of two particles in the neighborhood of the equilibrium. In the linear approximation, the interaction force and torque of (45) can be represented as

$$\begin{aligned} \mathbf{F} &= \sum_{k,n} \Psi(\xi_{kn}^0) \cdot (\xi_{kn} - \xi_{kn}^0), \quad \Psi(\xi) \stackrel{\text{def}}{=} \frac{d}{d\xi} \mathbf{f}(\xi) = 2\Phi'(\xi^2) \xi \xi + \Phi(\xi^2) \mathbf{E}, \\ \mathbf{M} &= \sum_{k,n} [(\xi_k^0 - \mathbf{r}_c) \times \Psi(\xi_{kn}^0) \cdot (\xi_{kn} - \xi_{kn}^0) - \xi_{kn}^0 \times \Psi(\xi_{kn}^0) \cdot (\xi_k - \xi_k^0)], \end{aligned} \quad (46)$$

where  $\xi_k^0$  and  $\xi_{kn}^0$  are the values of  $\xi_k$  and  $\xi_{kn}$  in the equilibrium. The difference between the current values and the equilibrium values of the vectors  $\xi_k$  and  $\xi_{kn}$  has the form

$$\xi_k - \xi_k^0 = \mathbf{r}_1 - \mathbf{r}_1^0 + \varphi_1 \times \rho_k, \quad \xi_{kn} - \xi_{kn}^0 = -\mathbf{r} + \mathbf{r}_0 + \varphi_1 \times \rho_k - \varphi_2 \times \rho_n, \quad (47)$$

where  $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$  is the vector from the center of mass of particle 1 to the center of mass of particle 2,  $\mathbf{r}_0$  is the equilibrium value of  $\mathbf{r}$ ,  $\varphi_1$  and  $\varphi_2$  are the vectors of small rotations of the particles, and  $\rho_k = \xi_k^0 - \mathbf{r}_1^0$  and  $\rho_n = \xi_n^0 - \mathbf{r}_2^0$  are the relative position vectors of point masses of particles 1 and 2, respectively, in the equilibrium. By substituting (47) into (46) and taking into account the equilibrium conditions

$$\sum_{k,n} \mathbf{f}(\xi_{kn}^0) \equiv \mathbf{0}, \quad \sum_{k,n} (\xi_k^0 - \mathbf{r}_c) \times \mathbf{f}(\xi_{kn}^0) \equiv \mathbf{0}, \quad (48)$$

one can represent the expressions for the force and the torque in the form of [7] that was obtained previously for a general interaction,

$$\mathbf{F} = \mathbf{A} \cdot \boldsymbol{\varepsilon} + \mathbf{B} \cdot \boldsymbol{\kappa}, \quad \mathbf{M} = \boldsymbol{\varepsilon} \cdot \mathbf{B} + \mathbf{C} \cdot \boldsymbol{\kappa}, \quad (49)$$

$$\boldsymbol{\varepsilon} = \mathbf{r} - \mathbf{r}_0 + \frac{1}{2} \mathbf{r}_0 \times (\varphi_1 + \varphi_2), \quad \boldsymbol{\kappa} = \varphi_2 - \varphi_1, \quad (50)$$

$$\mathbf{A} = - \sum_{k,n} \Psi(\xi_{kn}^0), \quad \mathbf{B} = \frac{1}{2} \sum_{k,n} \Psi(\xi_{kn}^0) \times (\rho_k + \rho_n), \quad (51)$$

$$\mathbf{C} = \frac{1}{2} \sum_{k,n} \left[ \frac{1}{2} \mathbf{r}_0 \times \Psi(\xi_{kn}^0) \times \mathbf{r}_0 + \rho_k \times \Psi(\xi_{kn}^0) \times \rho_n + \rho_n \times \Psi(\xi_{kn}^0) \times \rho_k \right].$$

Consider as an example a square crystal lattice whose atoms are modeled by point masses (Fig. 2a). If the atoms at the lattice points are assumed to interact only with the nearest atoms lying at the distance  $|\mathbf{a}_\alpha| = a$ , then the equilibrium



is neutral. However, the equilibrium configuration becomes unstable if the influence of the atoms located at the lattice points at the distance  $\sqrt{2}a$  is taken into account. We will analyze the origin of this mismatch. For the equilibrium configuration of the lattice to be stable, the expression of (37) for the internal energy must be positive definite. The linear terms occurring in this expression are unimportant, since the expression of (37) can be represented as the quadratic form

$$\rho U = \frac{1}{2} \varepsilon \cdot \cdot {}^4\mathbf{A}_* \cdot \cdot \varepsilon + \varepsilon \cdot \cdot {}^4\mathbf{B}_* \cdot \cdot \boldsymbol{\kappa} + \frac{1}{2} \boldsymbol{\kappa} \cdot \cdot {}^4\mathbf{C}_* \cdot \cdot \boldsymbol{\kappa}, \quad (52)$$

where  $\varepsilon$  and  $\boldsymbol{\kappa}$  differ from the respective quantities of (37) by certain constants. Therefore, the stability of the lattice is determined by the stiffness tensors  ${}^4\mathbf{A}_*$ ,  ${}^4\mathbf{B}_*$ , and  ${}^4\mathbf{C}_*$ . Regarding the atoms as point masses, we obtain

$$\mathbf{A}_\alpha = A \mathbf{e}_\alpha \mathbf{e}_\alpha, \quad \mathbf{B}_\alpha = \mathbf{0}, \quad \tilde{\mathbf{C}}_\alpha = \mathbf{0}, \quad \mathbf{e}_\alpha = \frac{\mathbf{a}_\alpha}{a_\alpha}, \quad (53)$$

where the coefficient  $A$  is determined by the potential of the interatomic interaction and depends on the distance between the atoms. The calculation of the stiffness tensors of (41) for the crystal lattice under consideration leads to

$${}^4\mathbf{A}_* = \frac{a^2}{V_*} [(A_1 + A_2)(\mathbf{e}_1 \mathbf{e}_1 + \mathbf{e}_2 \mathbf{e}_2) + A_2(\mathbf{e}_1 \mathbf{e}_2 + \mathbf{e}_2 \mathbf{e}_1 + \mathbf{e}_3 \mathbf{e}_3)], \quad {}^4\mathbf{B}_* = \mathbf{0}, \quad {}^4\mathbf{C}_* = \mathbf{0}, \quad (54)$$

$$\mathbf{e}_1 = \mathbf{i}\mathbf{i}, \quad \mathbf{e}_2 = \mathbf{j}\mathbf{j}, \quad \mathbf{e}_3 = \mathbf{i}\mathbf{j} + \mathbf{j}\mathbf{i},$$

where  $A_1$  and  $A_2$  are the values of the coefficient  $A$  of (53) that characterize the stiffness of the interaction with point masses located at the distances  $a$  and  $\sqrt{2}a$ , respectively. The unit vectors  $\mathbf{i}$  and  $\mathbf{j}$  are directed along the edges of the square lattice.

With reference to (54), one can express the internal energy density of (52) in the form

$$\rho U = \frac{1}{2} \varepsilon \cdot \cdot {}^4\mathbf{A}_* \cdot \cdot \varepsilon = \frac{a^2}{2V_*} [(A_1 + A_2)(\varepsilon_x^2 + \varepsilon_y^2) + 2A_2\varepsilon_x\varepsilon_y + A_2(\varepsilon_{xy} + \varepsilon_{yx})^2]. \quad (55)$$

The equilibrium condition of a crystal lattice consisting of point masses has the form  $\boldsymbol{\tau} = \mathbf{0}$ . Due to the symmetry, this tensor equation can be reduced to a single scalar equation  $\text{tr } \boldsymbol{\tau} = 0$ , which, in accordance with (20), can be written as follows:

$$\sum_{\alpha=1}^4 \mathbf{a}_\alpha \cdot \mathbf{F}_\alpha = 0. \quad (56)$$

If the interaction between the point masses is characterized by the potential  $\Pi(r)$ , then the equilibrium equation of (56) can be reduced to the form

$$\Pi'(a) + \sqrt{2}\Pi'(\sqrt{2}a) = 0. \quad (57)$$

Consider as an example, the Mie potential

$$\Pi(r) = \frac{D}{n-m} \left[ m \left( \frac{r_0}{r} \right)^n - n \left( \frac{r_0}{r} \right)^m \right], \quad n > m \geq 2, \quad (58)$$

where  $r_0$  is the distance between the point masses in the equilibrium and  $D$  is the depth of the potential well. From Eq. (57) one can calculate the equilibrium distance between the atoms of the crystal lattice,

$$a = \frac{r_0}{\sqrt{2}} \sqrt[n-m]{\frac{1 + \sqrt{2}^n}{1 + \sqrt{2}^m}}. \quad (59)$$

Using the relations of (58) and (59), one can calculate the elastic stiffness coefficients,  $A_1 = \Pi''(a)$  and  $A_2 = \Pi''(\sqrt{2}a)$ ,

$$A_1 = \frac{2Dnm}{r_0^2(n-m)} \sqrt[n-m]{\frac{(1 + \sqrt{2}^m)^{m+2}}{(1 + \sqrt{2}^n)^{n+2}}} [(n+1)\sqrt{2}^n - (m+1)\sqrt{2}^m + (n-m)\sqrt{2}^{m+n}], \quad (60)$$

$$A_2 = \frac{Dnm(n+1)(m+1)}{r_0^2(n-m)} \sqrt[n-m]{\frac{(1 + \sqrt{2}^m)^{m+2}}{(1 + \sqrt{2}^n)^{n+2}}} \left( \frac{1 + \sqrt{2}^m}{m+1} - \frac{1 + \sqrt{2}^n}{n+1} \right).$$

Simple analysis of the expressions of (60) shows that  $A_1 > 0$  for all  $m > 0$ , while  $A_2 < 0$  for  $m \geq 2$ . For negative  $A_2$ , the quadratic form of (55) is not positive definite and, hence, the configuration of the lattice is unstable. To neglect the influence of the second neighbors, one can set  $A_2 = 0$ . In this case, the equilibrium of the lattice becomes neutral, since the energy can be equal to zero for any strains  $\varepsilon_{xy}$  and  $\varepsilon_{yx}$ .

In what follows, we will show that by taking a generic particle to be the model of an atom one can provide the stability for the square crystal lattice. This is for that reason that when the torque interaction is taken into account, the transverse (shear) stiffness of interatomic interactions appears in addition to the longitudinal stiffness. The longitudinal stiffness characterizes the response to a change in the interatomic distance, whereas the transverse stiffness is due to the response of the system to the motion of the atoms in the direction perpendicular to the line connecting these atoms. As a result, when the particles reach a certain size, the transverse stiffness of the interaction with the nearest atoms can compensate for the negative transverse stiffness of the interaction with farther atoms and make the energy density positive definite.

Consider a square crystal lattice whose atoms are modeled by generic particles. Proceeding from the theory of symmetry of tensor quantities [7], one can show that if the symmetry type of the particles is identical to that of the square lattice, then the stiffness tensors that characterize the interaction between these particles have the form

$$\mathbf{A} = A\mathbf{e}_\alpha\mathbf{e}_\alpha + \tilde{A}\tilde{\mathbf{e}}_\alpha\tilde{\mathbf{e}}_\alpha, \quad \mathbf{B}_\alpha = \mathbf{0}, \quad \tilde{\mathbf{C}}_\alpha = \tilde{C}\mathbf{k}\mathbf{k}, \quad \mathbf{e}_\alpha = \frac{\mathbf{a}_\alpha}{|\mathbf{a}_\alpha|}, \quad \tilde{\mathbf{e}}_\alpha = \mathbf{k} \times \mathbf{e}_\alpha, \quad (61)$$

where  $\mathbf{k}$  is the unit vector normal to the lattice plane. The stiffness tensors of the crystal lattice,  ${}^4\mathbf{A}_*$ ,  ${}^4\mathbf{B}_*$ , and  ${}^4\mathbf{C}_*$ , and the stiffness tensors of the interatomic interactions of (61) are related by (39) and (41). Using these relations, we obtain

$$\begin{aligned} {}^4\mathbf{A}_* &= \frac{a^2}{V_*} [(A_1 + A_2 + \tilde{A}_2)(\mathbf{iiii} + \mathbf{jjjj}) + (\tilde{A}_1 + A_2 + \tilde{A}_2)(\mathbf{jiji} + \mathbf{ijij}) + (A_2 - \tilde{A}_2)(\mathbf{iiij} + \mathbf{jjii} + \mathbf{ijji} + \mathbf{jijj})], \\ {}^4\mathbf{B}_* &= \mathbf{0}, \quad {}^4\mathbf{C}_* = \frac{a^2}{V_*} (\tilde{C}_1 + 2\tilde{C}_2)(\mathbf{kiki} + \mathbf{kjkj}). \end{aligned} \quad (62)$$

Here coefficients  $A$ ,  $\tilde{A}$ , and  $\tilde{C}$  (defined in (61)) labeled with the indices  $\alpha = \pm 1, \pm 2$  characterize the stiffness of interaction with the atoms of the first coordination sphere, distanced by  $a$ , and ones labeled with the indices  $\alpha = \pm 3, \pm 4$  characterize the stiffness of interaction with the atoms of the second coordination sphere, distanced by  $\sqrt{2}a$ . The coefficients  $A$ ,  $\tilde{A}$ , and  $\tilde{C}$  correspond to the longitudinal stiffness (characterizing the response to a change in the distance between the atoms), the transverse (shear) stiffness, and the torsional stiffness (characterizing the response to a relative rotation of the particles). Substitute the expressions of (62) into the expression of (37) for the internal energy density (with the linear terms being omitted) to obtain

$$\begin{aligned} \rho U &= \frac{1}{2} \boldsymbol{\varepsilon} \cdot \cdot {}^4\mathbf{A}_* \cdot \cdot \boldsymbol{\varepsilon} + \frac{1}{2} \boldsymbol{\kappa} \cdot \cdot {}^4\mathbf{C}_* \cdot \cdot \boldsymbol{\kappa} = \frac{a^2}{2V_*} [(A_1 + A_2 + \tilde{A}_2)(\varepsilon_x^2 + \varepsilon_y^2) + 2(A_2 - \tilde{A}_2)\varepsilon_x\varepsilon_y \\ &\quad + (\tilde{A}_1 + A_2 + \tilde{A}_2)(\varepsilon_{xy}^2 + \varepsilon_{yx}^2) + 2(A_2 - \tilde{A}_2)\varepsilon_{xy}\varepsilon_{yx} + (\tilde{C}_1 + 2\tilde{C}_2)(\kappa_{zx}^2 + \kappa_{yz}^2)]. \end{aligned} \quad (63)$$

For the quadratic form of (63) to be positive definite, it is sufficient that

$$A_1 + A_2 + \tilde{A}_2 > |A_2 - \tilde{A}_2|, \quad \tilde{A}_1 + A_2 + \tilde{A}_2 > |A_2 - \tilde{A}_2|, \quad \tilde{C}_1 + 2\tilde{C}_2 > 0. \quad (64)$$

Specific values of the stiffness coefficients of the atoms of the lattice ( $A_\gamma$ ,  $\tilde{A}_\gamma$ , and  $\tilde{C}_\gamma$ ) depend on the potential of the interaction. For a potential which fairly rapidly decays and has a structure similar to that of the Mie potential, one can readily show that (i) the longitudinal and torsional stiffnesses of interaction with the atoms of the first coordination sphere are positive, while the transverse stiffness can be either positive or negative, (ii) all stiffnesses characterizing the interaction with the atoms of the second coordination sphere are negative, i.e.,

$$A_1 > 0, \quad \tilde{A}_1 \geq 0, \quad \tilde{C}_1 > 0, \quad A_2 < 0, \quad \tilde{A}_2 < 0, \quad \tilde{C}_2 < 0, \quad (65)$$

(iii) the transverse stiffnesses are substantially less than the corresponding longitudinal stiffnesses,

$$|\tilde{A}_1| \ll A_1, \quad |\tilde{A}_2| \ll |A_2|, \quad (66)$$

and (iv) the stiffnesses of interaction with the farther atoms are substantially less than the corresponding stiffnesses of interaction with the nearest atoms,

$$|A_2| \ll |A_1|, \quad |\tilde{A}_2| \ll |\tilde{A}_1|, \quad |\tilde{C}_2| \ll |\tilde{C}_1|. \quad (67)$$

If the relations of (65)–(67) hold, then the first and third inequalities of (64) hold automatically, and the second inequality becomes

$$\tilde{A}_1 > 2|A_2|. \quad (68)$$

The condition of (68) has a simple physical meaning — the transverse stiffness of interaction with the atoms of the first coordination sphere must exceed the doubled absolute value of the stiffness of interaction with the atoms of the second coordination sphere.

As a simple model of particles that enables one to take into account the symmetry of the lattice, consider particles that consist of four point masses rigidly connected to each other and located at the vertices of a square (Fig. 2b). Let the length of the side of the square be  $h$ . Select a primary particle, label it with  $\alpha = 0$ , and consider the interaction of this particle with the neighboring particles labeled with  $\alpha = \pm 1, \pm 2, \pm 3, \pm 4$  (Fig. 2a). The particles with  $\alpha = \pm 1$  and  $\alpha = \pm 2$  are turned to each other and to the primary particle with sides and are distanced by  $a$ . The particles with  $\alpha = \pm 3$  and  $\alpha = \pm 4$  are turned to each other and to the primary particle with vertices and are distanced by  $\sqrt{2}a$ . The equilibrium conditions for the crystal lattice are  $\tau = \mathbf{0}$  and  $\mu = \mathbf{0}$ . These conditions are equivalent to one scalar equation  $\text{tr } \tau = 0$ , since the other equations hold identically due to the symmetry of the lattice. In accordance with (20), the equation  $\text{tr } \tau = 0$  can be represented in the form of (56). We will assume that the interaction between the point masses belonging to different particles is defined by the potential  $\Pi(r)$ . Then the equilibrium equation of (56) becomes

$$\sum_{\gamma=1}^2 (\sqrt{2})^{\gamma-1} \left[ \sum_{i=1}^3 \nu_{i\gamma} \Pi'(r_{i\gamma}) + \nu_{4\gamma} \Pi'(r_{i\gamma}) \frac{\xi_{1\gamma}}{\xi_{4\gamma}} + \sum_{i=5}^6 \nu_{i\gamma} \Pi'(r_{i\gamma}) \frac{1}{\xi_{i\gamma}} \left( \frac{1}{\gamma} \xi_{i-3,\gamma} + \frac{\gamma-1}{2} \xi_{i\gamma} \right) \right] = 0, \quad (69)$$

$$\xi_{1\gamma} = \sqrt{\gamma}, \quad \xi_{2\gamma} = \sqrt{\gamma}(1 + \zeta), \quad \xi_{3\gamma} = \sqrt{\gamma}(1 - \zeta), \quad \xi_{4\gamma} = \sqrt{\gamma}\sqrt{1 + \zeta^2},$$

$$\xi_{5\gamma} = \sqrt{\gamma} \sqrt{\left(1 + \frac{\zeta}{\gamma}\right)^2 + \left(\frac{\zeta}{\gamma}\right)^2}, \quad \xi_{6\gamma} = \sqrt{\gamma} \sqrt{\left(1 - \frac{\zeta}{\gamma}\right)^2 + \left(\frac{\zeta}{\gamma}\right)^2}, \quad \zeta = \frac{h}{a},$$

$$r_{i\gamma} = a\xi_{i\gamma}, \quad \nu_{1\gamma} = 2, \quad \nu_{2\gamma} = \nu_{3\gamma} = \frac{1}{\gamma}, \quad \nu_{4\gamma} = \frac{2}{\gamma}, \quad \nu_{5\gamma} = \nu_{6\gamma} = \gamma,$$

where  $\gamma = 1$  for the particles turned to one another with their sides and  $\gamma = 2$  for the particles turned to one another with their vertices. Using the relations of (51), one can readily show that the stiffness tensors  $\mathbf{A}_\alpha$ ,  $\mathbf{B}_\alpha$ , and  $\tilde{\mathbf{C}}_\alpha$ , characterizing the interaction between the particles, have the form of (61), where the elastic coefficients  $A_\gamma$ ,  $\tilde{A}_\gamma$ , and  $\tilde{C}_\gamma$  are expressed in terms of the potential  $\Pi(r)$  as follows:

$$\begin{aligned} A_\gamma &= 2 \sum_{i=1}^6 \nu_{i\gamma} c_{i\gamma} - \tilde{A}_\gamma, & \tilde{A}_\gamma &= 2\zeta^2 \sum_{i=4}^6 \frac{\nu_{i\gamma} c_{i\gamma}}{\xi_{i\gamma}^2}, \\ C_\gamma &= a^2 \zeta^2 \left[ c_{1\gamma} + \left(1 - \frac{\gamma}{2}\right) \sum_{i=2}^3 c_{i\gamma} + \frac{(2-\gamma)c_{4\gamma}\zeta^2}{\xi_{4\gamma}^2} + \frac{\gamma-1}{2} \sum_{i=5}^6 \frac{c_{i\gamma}\xi_{i-3,\gamma}}{\xi_{i\gamma}^2} \right], \\ \tilde{C}_\gamma &= C_\gamma + \frac{\gamma a^2 \tilde{A}_\gamma}{4}, & c_{i\gamma} &= \Pi''(r_{i\gamma}) - \frac{\Pi'(r_{i\gamma})}{r_{i\gamma}}, \quad r_{i\gamma} = a\xi_{i\gamma}. \end{aligned} \quad (70)$$

In what follows, we will assume that the interaction between the mass points is described by the Mie potential. In this case, Eq. (69) has an exact closed-form solution which expresses the equilibrium distance  $a$  in terms of the dimensionless parameter  $\zeta = h/a$ ,

$$\left(\frac{a}{r_0}\right)^{n-m} = \frac{\sum_{\gamma=1}^2 (\sqrt{2})^{\gamma-1} \left[ \sum_{i=1}^3 \frac{\nu_{i\gamma}}{\xi_{i\gamma}^{-(n+1)}} + \frac{\nu_{4\gamma}\xi_{1\gamma}}{\xi_{4\gamma}^{-(n+2)}} + \sum_{i=5}^6 \frac{\nu_{i\gamma}}{\xi_{i\gamma}^{-(n+1)}} \left( \frac{1}{\gamma} \xi_{i-3,\gamma} + \frac{\gamma-1}{2} \xi_{i\gamma} \right) \right]}{\sum_{\gamma=1}^2 (\sqrt{2})^{\gamma-1} \left[ \sum_{i=1}^3 \frac{\nu_{i\gamma}}{\xi_{i\gamma}^{-(m+1)}} + \frac{\nu_{4\gamma}\xi_{1\gamma}}{\xi_{4\gamma}^{-(m+2)}} + \sum_{i=5}^6 \frac{\nu_{i\gamma}}{\xi_{i\gamma}^{-(m+1)}} \left( \frac{1}{\gamma} \xi_{i-3,\gamma} + \frac{\gamma-1}{2} \xi_{i\gamma} \right) \right]}. \quad (71)$$

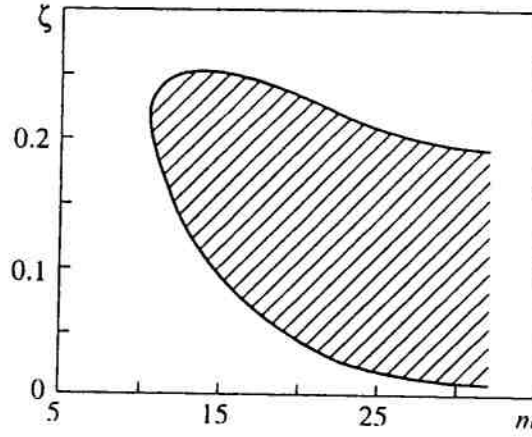


Fig. 3

The elastic coefficients  $c_{i\gamma}$  that characterize the interaction of the mass points belonging to different particles (see the relations of (70)) can be expressed in terms of the parameters of the Mie potential as follows:

$$c_{i\gamma} = \frac{Dnm}{r_0^2(n-m)} \left( \frac{r_0}{a} \right)^{n+2} \left[ \frac{n+2}{\xi_{i\gamma}^{n+2}} - \left( \frac{a}{r_0} \right)^{n-m} \frac{m+2}{\xi_{i\gamma}^{m+2}} \right]. \quad (72)$$

By substituting the expressions of (69), (71), and (72) into the relations of (70) for the elastic coefficients  $A_\gamma$ ,  $\tilde{A}_\gamma$ , and  $\tilde{C}_\gamma$ , one can verify that the stability conditions of (64) depend on three parameters,  $m$ ,  $n$ , and  $\zeta$ . The first two parameters determine the rate of decay of the Mie potential. The parameter  $\zeta = h/a$  is the ratio of the size of the particle to the interatomic distance.

The results of the numerical analysis of the stability conditions of (64) for the crystal lattice are presented in Fig. 3. This figure shows the stability region (shaded) on the plane of the parameters  $\zeta$  and  $m$ . The parameters of the Mie potential were assumed to satisfy the relation by  $n = 2m$ . It is apparent that for small  $m$ , when the rate of decay of the interaction potential is not high enough and the destabilizing role of the farther neighbors is significant, the lattice is unstable for any sizes of the particles. An increase in  $m$  leads to the appearance of the stability region. As has been mentioned previously, for the stability to be provided, the transverse stiffness of interaction with the neighboring atoms,  $\tilde{A}_1$ , must exceed the doubled absolute value of the longitudinal stiffness of interaction with the farther atoms,  $A_2$ . (See (68).) If  $\zeta$  is regarded as a small quantity, the longitudinal stiffness has an order of unity and the transverse stiffness has an asymptotic order of  $\zeta^2$ ; see (70). Therefore, the lower boundary of the stability region can be accounted for by the fact that for the stability to be ensured the size of the particles must exceed a certain value  $\zeta_*(n, m)$ . Since  $|A_2|$  decreases as  $m$  and  $n$  increase, the value of  $\zeta_*(n, m)$  also decreases with the increase of these parameters. The upper boundary of the stability region is due to the fact that the transverse stiffness of the interaction with the nearest atoms,  $\tilde{A}_1$ , becomes a decreasing function, starting with some  $\zeta$ , and is negative for sufficiently large  $\zeta$ .

We will summarize the most important results obtained in this paper.

1. We have introduced the concept of strain vectors for a system of two interacting particles. We have shown that the strain vectors defined as the vectors on which the interaction force and torque perform work cannot be unambiguously introduced for a discrete system. This is for that reason that the torque of the interaction between the particles depends on the point with respect to which this torque is calculated and the choice of this point in a discrete system is ambiguous. We have compared this situation with a similar situation in continuous systems.

2. We have shown that the dynamics of a crystal packing of particles with rotational degrees of freedom in the long-wave approximation is described by the equations of macroscopic couple stress elasticity. Specific expressions have been obtained for the stiffness tensors of a crystal lattice. These tensors depend on the geometrical parameters of the lattice and the stiffness tensors of rank 2 which characterize the stiffness of the interatomic interaction.

3. As an example of a generic particle we have considered the particles consisting of point masses rigidly attached to one another. The interaction between the point masses belonging to different particles is characterized by a pairwise potential. The expressions for the stiffness tensors of rank 2 that characterize the stiffness of interaction between two identical particles have been obtained.

4. We have shown that one can stabilize a square crystal lattice by using generic particles as a model of the atoms forming the particle. A simple model of the particle has been proposed to take into account the symmetry of the square

lattice. This model involves four point masses that lie at the vertices of a square and are rigidly connected to one another. For this model, stability regions of the lattice have been identified. These stability regions depend on the ratio of the size of the particle to the equilibrium interatomic distance and the parameters of the interaction potential.

The models of the particles located at the nodal points of the square lattice can be rather diverse. The only requirement to be met is that the symmetry type of the particle should be matched with that of the lattice. A criterion for selection of a model can be, on the one hand, the simplicity of this model and, on the other hand, the degree to which this model reflects the structure of the atom. In this paper, we preferred the simplicity criterion. To take into account the structure of the atom, one could modify the primary model as follows: One could place a point mass at the center of the square to model the nucleus and regard the point masses at the vertices of the square as electrons. In such an interpretation, it is reasonable to assume the potentials of nucleus-nucleus, nucleus-electron, and electron-electron interactions to be different. This will result in a model with a large number of parameters. This model does not possess an advantage of simplicity and, for this reason, it is difficult to assess the adequacy of this model, since by varying a large number of parameters one can always achieve good agreement with experimental data. An alternative approach consists in modeling atoms by generic particles without specifying its structure as a set of point masses. An advantage of this approach is that it does not imply an attempt to take into account the structure of the atom. The parameters characterizing the interaction between the generic particles are completely determined by the structure of the lattices that can be formed by these particles. An implementation of this approach requires the creation of the interaction potentials that depend not only on the relative position of the particles but also on their relative orientation. In the linear formulation, the interaction potential for generic particles has the form of (6). The nonlinear formulation of the problem needs a separate study and leads beyond the scope of this paper.

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St. Petersburg