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MECHANICS

Inclusion of the Moment Interaction in the Calculation of the Flexural Rigidity of Nanostructures

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In recent years, in addition to the investigation of the electronic and optical properties of nanostructures [1], the study of their mechanical properties has become particularly important. Many works have been devoted to the production of nanotubes and investigation of their properties [2–8]. According to the data obtained in [4], nanotubes can retain their elastic properties under significant strains. The stress–strain state of nanotubes is usually calculated in the theory of elastic shells [9]. In this case, the elastic moduli are determined in discrete models, where only the force interaction between atoms forming a nanotube is taken into account. However, the existence of monolayer nanotubes [5–8] makes it necessary to consider also the moment interaction between atoms. Otherwise, the atomic layer forming the nanotube would have zero flexural rigidity, so that such a nanotube would be unstable.

The aim of this study is the development of a method of determining the flexural rigidity of nanostructures with allowance for the moment interaction on the nanolevel. First, we obtain general formulas for the moment interaction between atoms or molecules. Then, we apply these formulas to the discrete model [10, 11] to obtain the corrections associated with the moment interaction. These corrections make it possible to describe the mechanical properties of monolayer nanostructures.

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We consider a crystal consisting of particles (atoms or molecules) whose interaction depends not only on their mutual arrangement in space but also on their mutual orientation. This interaction is characterized by the force vector and moment vector. The force and moment of the interaction between crystal particles are defined according to the theory of shells and rods [12, 13]. We consider two interacting particles (Fig. 1). In the actual configuration, the positions and orientations of the particles are specified by the radius-vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ and rotation vectors $\boldsymbol{\varphi}_1$ and $\boldsymbol{\varphi}_2$, respectively. In the equilibrium position, $\mathbf{r}_2 - \mathbf{r}_1 = \mathbf{r}_0$, $\boldsymbol{\varphi}_1 = 0$, and $\boldsymbol{\varphi}_2 = 0$. Let us introduce the following notation: $\mathbf{F}_1$ and $\mathbf{M}_1$ are the force and moment, respectively, acting on particle 1 by particle 2; $\mathbf{F}_2$ and $\mathbf{M}_2$ are the force and moment, respectively, acting on particle 2 by particle 1; and $\mathbf{F}_i^{\mathrm{e}}$ and $\mathbf{M}_i^{\mathrm{e}}$ are the external forces and moments, respectively, acting on the ith particle. The moments $\mathbf{M}_i$ and $\mathbf{M}_i^{\mathrm{e}}$ are calculated with respect to the ith particle. Following the moment theory of elasticity [14], we write the equations of motion for particle 1, particle 2, and the system including both particles in the form

$$\begin{aligned}
m_1\dot{\mathbf{v}}_1 &= \mathbf{F}_1 + \mathbf{F}_1^{\mathrm{e}}, \quad (\theta_1 \cdot \boldsymbol{\omega}_1)^{\cdot} = \mathbf{M}_1 + \mathbf{M}_1^{\mathrm{e}},\\
m_2\dot{\mathbf{v}}_2 &= \mathbf{F}_2 + \mathbf{F}_2^{\mathrm{e}}, \quad (\theta_2 \cdot \boldsymbol{\omega}_2)^{\cdot} = \mathbf{M}_2 + \mathbf{M}_2^{\mathrm{e}},\\
(m_1\mathbf{v}_1 + m_2\mathbf{v}_2)^{\cdot} &= \mathbf{F}_1^{\mathrm{e}} + \mathbf{F}_2^{\mathrm{e}},\\
(\mathbf{r}_1 \times m_1\mathbf{v}_1 + \theta_1 \cdot \boldsymbol{\omega}_1 + \mathbf{r}_2 \times m_2\mathbf{v}_2 + \theta_2 \cdot \boldsymbol{\omega}_2)^{\cdot}&\\
= \mathbf{r}_1 \times \mathbf{F}_1^{\mathrm{e}} + \mathbf{M}_1^{\mathrm{e}} + \mathbf{r}_2 \times \mathbf{F}_2^{\mathrm{e}} + \mathbf{M}_2^{\mathrm{e}}.&
\end{aligned} \tag{1}$$

Here, m_1 and m_2 are the masses of the particles, θ_1 and θ_2 are their inertia tensors, $\mathbf{v}_1$ and $\mathbf{v}_2$ are the velocities of the particles, and $\boldsymbol{\omega}_1$ and $\boldsymbol{\omega}_2$ are their angular velocities. We emphasize that the moment balance equation in a system of bodies, in contrast to a system of material points, does not result from the force balance equation. These equations are independent laws. Newton's third

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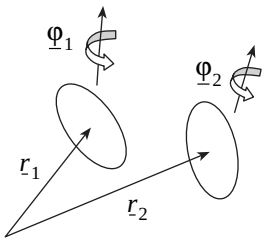

Fig. 1. Moment interaction between two particles.

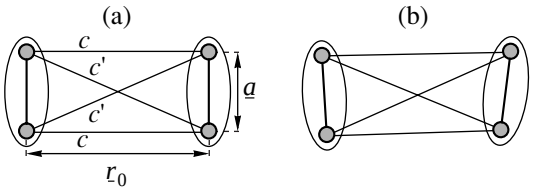

Fig. 2. Two interacting particles: (a) reference (equilibrium) position and (b) actual position.

law for forces and its analogue for moments follow from Eqs. (1):

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

The energy balance equation for the two-particle system is written in the form

$$\left(\frac{1}{2}[m_1\mathbf{v}_1 \cdot \mathbf{v}_1 + \boldsymbol{\omega}_1 \cdot \theta_1 \cdot \boldsymbol{\omega}_1 + m_2\mathbf{v}_2 \cdot \mathbf{v}_2 + \boldsymbol{\omega}_2 \cdot \theta_2 \cdot \boldsymbol{\omega}_2] + U\right)^{\cdot} = \mathbf{F}_1^e \cdot \mathbf{v}_1 + \mathbf{M}_1^e \cdot \boldsymbol{\omega}_1 + \mathbf{F}_2^e \cdot \mathbf{v}_2 + \mathbf{M}_2^e \cdot \boldsymbol{\omega}_2, \quad (3)$$

where U is the internal energy of the system (the energy of interaction between particles 1 and 2). For small displacements from the equilibrium position in view of Eqs. (1) and (2), energy balance equation (3) reduces to the form

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

Here, $\mathbf{M}$ is the moment acting on particle 1 by particle 2 about the middle of the segment connecting these particles. The vectors $\boldsymbol{\varepsilon}$ and $\boldsymbol{\kappa}$ on which the force and moment, respectively, do work [see formulas (4)] are referred to as deformation vectors. In what follows, we discuss the elastic deformation of the system. We assume that the internal energy, force, and moment depend only on the deformation vectors and are independent of the velocities. Then,

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

We assume that the internal energy is a quadratic form of the deformation vectors

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

The coefficients of quadratic form (6) are called the elasticity tensors. In the linear theory of elasticity, the elasticity tensors are constants such that the tensors A and C are symmetric, while the tensor B is arbitrary. According to formulas (5) and (6), the force and moment have the form

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

For illustration, we consider the simplest model of the moment interaction, where any particle is simulated by two rigidly bound material points (Fig. 2). The following notation is used: $\mathbf{a}$ is the vector connecting two material points within one particle and $\mathbf{r}_0$ is the vector specifying the equilibrium distance between different particles. Both vectors correspond to the reference (equilibrium) configuration for the two-particle system (Fig. 2a). The actual configuration of the system is shown in Fig. 2b. The interaction between material points belonging to different particles is described by the pure force interaction (the rigidities of the corresponding bonds are denoted as c and c'). However, the total interaction between particles has both force and moment components. In Fig. 2, the quantity a characterizes the arm of the moment interaction. When $a \longrightarrow 0$, the moment interaction transforms to the pure force interaction. Calculation of the force and moment acting on particle 1 by particle 2 showed that these quantities have form (7), where

$$\begin{aligned} A &= C_1\mathbf{ii} + C_1^*\mathbf{jj}, \quad B = 0, \quad C = C_2\mathbf{kk}, \\ \mathbf{i} &= \frac{\mathbf{r}_0}{|\mathbf{r}_0|}, \quad \mathbf{j} = \frac{\mathbf{a}}{a}, \quad \mathbf{k} = \mathbf{i} \times \mathbf{j}, \\ C_1 &= 2(c + c'\cos^2\alpha), \\ C_1^* &= 2c'\sin^2\alpha, \quad C_2 = \frac{ca^2}{2}, \quad \tan\alpha = \frac{\alpha}{r_0}. \end{aligned} \quad (8)$$

As a rule, atoms in a nanocrystal are simulated by material points. The simulation of nanocrystal atoms by particles with rotational degrees of freedom complicates the theory of the interaction between particles. However, this complication is justified, because it enables one to describe a number of physical effects that can be described only by multiparticle interaction

potentials in a system of material points [8, 15]. In particular, the class of stable crystal lattices is extended. At the same time, formulations of problems in the theory of moment interactions are much simpler than those in the approach using multiparticle potentials. As is shown below, the inclusion of the moment interactions makes it possible to find an analytical expression for the flexural rigidity of a nanocrystal that does not vanish when the crystal consists of a single atomic layer.

As an example, we apply moment theory to the model problem of the bending of a nanocrystalline strip [10, 11]. We consider a two-dimensional single crystal composed of N and K layers in the y and x directions, respectively, so that $K \gg N$ (Fig. 3). For the force and moment characterizing the interaction between particles, we will use expressions (7), where the elasticity tensors are represented in the form

$$A = C_1\frac{\mathbf{r}_0\mathbf{r}_0}{|\mathbf{r}_0|^2} + C_1^*\frac{\mathbf{k}\times\mathbf{r}_0\mathbf{k}\times\mathbf{r}_0}{|\mathbf{r}_0|^2}, \quad B = 0, \quad C = C_2\mathbf{k}\mathbf{k}. \tag{9}$$

Here, $\mathbf{k}$ is the unit vector perpendicular to the strip plane. The coefficients C_1, C_1^*, and C_2 depend on the structure and sizes of interacting particles. Formulas (9) present the general form of the tensors A, B, and C in the plane problem provided that the system consisting of two interacting particles has two mutually perpendicular symmetry axes. This conclusion can be easily proved by using the symmetry theory of tensors [12].

In this study, we consider only a triangular crystal lattice. The particles that are described by relationships (9) and satisfy the symmetry of a triangular lattice can be simulated by a set of six material points situated at the vertices of a regular hexagon. However, below, we will use general relationship (9) disregarding the internal structure of a particle. For clarity, particles will be represented as ovals, which makes it possible to show their relative rotations (Fig. 3).

The particles located at crystal sides are subjected to the forces Q_j (Fig. 3) varying linearly when going from one layer to another such that the total load is purely moment:

$$\sum_{j=1}^{N} Q_j = 0, \quad \sum_{j=1}^{N} R_j Q_j = M_\Sigma. \tag{10}$$

It is assumed that particles on the crystal sides cannot rotate about each other; i.e., the crystal sides rotate as a rigid body. Only interactions between an atom and its nearest neighbors in the crystal lattice are taken into account (Fig. 3). The strain state of the crystal is determined by the distances $a_{i,j}$ between neighboring atoms in each layer, the distances $b_{i,j}$ between the nearest atoms in the neighboring layers, and the rotation angles $\varphi_{i,j}$ of the atoms. The indices i and j correspond to the numbers of layers in the x and y directions, respectively

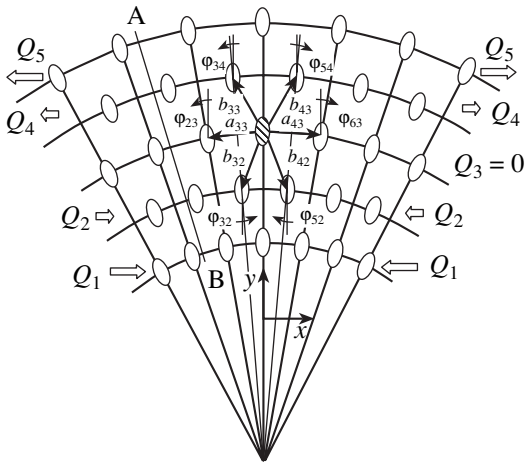

Fig. 3. Bending of the nanocrystalline strip.

(Fig. 3). The distances between the neighboring layers are determined from the relationship $h_{i,j}^2 = b_{i,j}^2 - \frac{a_{i,j}^2}{4}$. In the undeformed state, the crystal lattice consists of equilateral triangles with the side $a = b = a_0$; the rotation angles $\varphi_{i,j}$ of the atoms are assumed to be equal to zero. It is easy to check that, in the undeformed state, the relationships $h_0 = \frac{\sqrt{3}a_0}{2}$, and $R_j = (j-1)h_0$, where R_j is the distance between the jth and first atomic layers, are valid. Writing the equilibrium equations for the atoms, we arrive at the system of equations whose solution has the form

$$\Delta b_{i,j} = 0, \quad \Delta a_{i,j} = \frac{4\sqrt{3}M_\Sigma(2j-N-1)}{C_1 a_0(N-1)N(N+1)}, \quad \varphi_{i,j} = (i-1)\alpha, \quad \alpha = \frac{\frac{\Delta a_{i,N}}{2} - \frac{\Delta a_{i,1}}{2}}{h_0(N-1)}. \tag{11}$$

It is seen from relationships (11) that, under the deformation of the crystal, the layers of atoms in the y direction remain rectilinear, the angles between any neighboring atomic layers are identical, and the rotation angles of the atoms coincide with those of the corresponding layers. Since the problem of pure bending is considered, the shear strain is equal to zero. Thus, the coefficient C_1^* characterizing the shear rigidity is absent in the solution of the problem and cannot therefore affect the flexural rigidity.

To determine the flexural rigidity of a single crystal strip, we mentally cut the crystal by a vertical straight line AB (Fig. 3). According to formulas (11), the total normal force acting from one part of the crystal to

another is equal to zero, and the total bending moment M^* has the form

$$M^* = M_\Sigma + C_2\alpha(3N-1). \quad (12)$$

The flexural rigidity is defined as the ratio of the moment M^* to the curvature β:

$$D \stackrel{\text{def}}{=} \frac{M^*}{\beta}, \quad \beta = \frac{2\alpha}{a_0}. \quad (13)$$

The substitution of formulas (11) and (12) into Eq. (13) gives

$$D = \frac{C_1 a_0^3}{16}(N-1)N(N+1) + \frac{C_2 a_0}{2}(3N-1). \quad (14)$$

The first term in (14) coincides with the formula for the flexural rigidity obtained in [11], where a similar problem was considered disregarding moment interactions between crystal particles. The second term is the correction caused by the moment interaction between the particles. The first term in formula (14) for $N = 1$ vanishes so that the flexural rigidity is completely determined by the quantity C_2 characterizing the moment interactions between crystal atoms

$$N = 1: \quad D = C_2 a_0. \quad (15)$$

When $N \longrightarrow \infty$, the second term in Eq. (14) becomes negligibly small compared to the first term, and the first term tends to the value taken in the macroscopic theory of plates

$$N \to \infty: \quad D \to D_\infty = \frac{E_\infty H^3}{12}, \quad E_\infty = \frac{2C_1}{\sqrt{3}}, \quad (16)$$

where E_∞ is the Young modulus of the infinite crystal and $H \stackrel{\text{def}}{=} Nh_0$ is the macroscopic thickness of the strip.

Thus, in this study, we found the general formulas describing the moment interaction between atoms or molecules under linear elastic deformation. These formulas are illustrated in application to the simplified problem of the bending of a two-dimensional nanocrystalline strip. However, these formulas can be similarly used in the general three-dimensional formulation. In addition, it is shown that, by including the moment interaction on the nanolevel, the elastic deformation of mono- and multilayer nanostructures can be commonly described, and the correction to the flexural rigidity that is nonzero for monolayer nanoobjects can be calculated.

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REFERENCES

1. N. N. Ledentsov, V. M. Ustinov, V. A. Shchukin, *et al.*, Fiz. Tekh. Poluprovodn. (St. Petersburg) **32** (4), 385 (1998) [Semiconductors **32**, 343 (1998)].
2. V. Ya. Prinz, A. V. Chekhovskiy, V. V. Preobrazhenskiĭ, *et al.*, Nanotechnology **21** (2), 231 (2002).
3. A. V. Maslov, É. N. Korytkova, and V. V. Gusarov, in *Proceedings of 4th International Symposium on Mineralogical Museum, St. Petersburg, 2002*, p. 286.
4. T. Kizuka, Phys. Rev. B: Condens. Matter **59**, 4646 (1999).
5. L.-M. Peng, Z. L. Zhang, Z. Q. Xue, *et al.*, Phys. Rev. Lett. **85**, 3249 (2000).
6. J.-P. Salvetat, G. A. D. Briggs, J.-M. Bonard, *et al.*, Phys. Rev. Lett. **82**, 944 (1999).
7. Y. H. Lee, S. G. Kim, and D. Tomanek, Phys. Rev. Lett. **78**, 2393 (1997).
8. P. Zhang, Y. Huang, H. Gao, and K. C. Hwang, ASME Trans. J. Appl. Mech. **69**, 454 (2002).
9. C. Q. Ru, Phys. Rev. B: Condens. Matter **62**, 9973 (2000).
10. A. M. Krivtsov and N. F. Morozov, Dokl. Akad. Nauk **381**, 345 (2001) [Dokl. Phys. **46**, 825 (2001)].
11. E. A. Ivanova, A. M. Krivtsov, and N. F. Morozov, Dokl. Akad. Nauk **385**, 494 (2002) [Dokl. Phys. **47**, 620 (2002)].
12. P. A. Zhilin, Tr. Leningr. Politekh. Inst. im. M. I. Kalinina **386**, 29 (1982).
13. P. A. Zhilin, A. D. Sergeeva, and T. P. Tovstik, in *Proceedings of 24th All-Russia School-Seminar on Analysis and Synthesis of Nonlinear Mechanical Oscillatory Systems, St. Petersburg, 1996* (1997), p. 313.
14. W. Nowacki, *Theory of Elasticity* (PWN, Warszawa, 1970; Mir, Moscow, 1975).
15. J. Tersoff, Phys. Rev. B: Condens. Matter **37**, 6991 (1988).

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