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ON THE DETERMINATION OF THE FLEXURAL RIGIDITY OF NANOSHELLS

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In view of the development of nanotechnologies, the problem of determining the mechanical characteristics of objects of the nanometer-size scale level becomes quite topical. Most theoretical investigations in this field are based on the use of equations of the macroscopic theory of elasticity. However, numerous researchers have noted a difference between the values of moduli of elasticity obtained from micro- and macroexperiments. The present work is devoted to the development of theoretical foundations for the experimental determination of the flexural rigidity of nanoshells.

Numerous researchers have noted a discrepancy between the values of moduli of elasticity obtained from micro- and macroexperiments. The dependence of the values of Young's modulus and flexural rigidity on the number of atomic layers of a single crystal was studied theoretically in [1, 3] on the example of a two-dimensional single-crystal strip. Comparison of the results [1, 3] shows that three expressions for flexural rigidity, namely, (i) the relation known from the continual theory, (ii) the expression obtained by substituting Young's modulus, calculated from the discrete model [3], in the formula of the continual theory, and (iii) the relation obtained directly from the discrete model [1], differ substantially for small numbers of atomic layers. Hence, the use of relations of the continual theory, ignoring the discrete properties of the material in the direction of nanoobject thickness, can lead to significant errors. At the same time, it is clear that taking the discrete properties into account becomes inessential for those directions where the number of atomic layers is large. Therefore, most likely, the use of continual equations is admissible for the numerical analysis of nanoobjects. Thus, the development of a method for the direct determination of flexural rigidity without using any formulas relating it to the nanoobject thickness and Young's modulus of the material represents an important problem. In [2], a study of the dynamics of cylindrical spiral nanoshells [4, 5] was carried out, and, on this basis, a procedure was developed for the experimental verification of applicability of the continual theory for calculations of nanometer-size objects, and a method was proposed for the experimental determination of the flexural rigidity of nanoshells. The main difficulty arising inevitably in the realization of the method proposed in [2] consists of fastening of the nanoobject. The engineering problem is connected here with fastening of the nanoobject in such a way that the measured frequencies should be really the natural vibration frequencies of the specimen under study but not of the microobject on which the specimen is fastened. To avoid these technical difficulties, one can apply the procedure described in what follows and based on the analysis of natural vibrations of a nanoobject on a substrate.

Basic Equations of the Theory of Elastic Shells

We give here a list of the basic equations of the classical linear theory of shells (for brevity, we use the apparatus of direct tensor calculus):

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$$\nabla \cdot \underline{\underline{T}} = \rho \frac{d^2 \underline{u}}{dt^2}, \qquad \nabla \cdot \underline{\underline{M}} + \underline{\underline{T}}_{\times} = 0,$$

$$\underline{\underline{T}} \cdot \underline{\underline{a}} + \frac{1}{2}(\underline{\underline{M}} \cdot\cdot \underline{\underline{b}}) \underline{\underline{c}} = {}^4\underline{\underline{A}} \cdot\cdot \underline{\underline{\varepsilon}}, \qquad \underline{\underline{M}}^{\top} = {}^4\underline{\underline{C}} \cdot\cdot \underline{\underline{\kappa}},$$

$$\underline{\underline{\varepsilon}} = \frac{1}{2}((\nabla \underline{u}) \cdot \underline{\underline{a}} + \underline{\underline{a}} \cdot (\nabla \underline{u})^{\top}), \qquad \underline{\underline{\kappa}} = (\nabla \underline{\varphi}) \cdot \underline{\underline{a}} + \frac{1}{2}((\nabla \underline{u}) \cdot\cdot \underline{\underline{c}}) \underline{\underline{b}},$$

$$\underline{\varphi} = -\underline{n} \times (\nabla \underline{u}) \cdot \underline{n}, \qquad \underline{\underline{b}} = -\nabla \underline{n}, \qquad \underline{\underline{c}} = -\underline{\underline{a}} \times \underline{n}. \tag{1}$$

Here, $\underline{\underline{T}}$ and $\underline{\underline{M}}$ are the force and momentum tensors, the vector invariant of a tensor is denoted by sign $(\cdot)_{\times}$, ρ is the surface density of mass, $\underline{u}$ is the displacement vector, $\underline{\varphi}$ is the vector of rotation angles, $\underline{\underline{\varepsilon}}$ is the tensor of tension-shearing strain in the tangential plane, $\underline{\underline{\kappa}}$ is the tensor of bending-torsion strain, ${}^4\underline{\underline{A}}$ and ${}^4\underline{\underline{C}}$ are the tensors of shell rigidity, $\underline{n}$ is the vector of unit normal to the shell surface, and $\underline{\underline{a}}$ is the unit tensor in the tangential plane.

Flexural Vibrations of a Cylindrical Shell

Consider a cylindrical shell of radius R. In the description of its kinematics, we use a cylindrical coordinate system $r \equiv R$, θ, z. As is well known, the tensor of shell rigidity in tension and shear in the tangential plane ${}^4\underline{\underline{A}}$ is proportional to the shell thickness h, but the tensor of rigidity in bending and torsion ${}^4\underline{\underline{C}}$ is proportional to h^3. Hence, in the case $h/R \ll 1$, we may consider the shell under study as inextensible. Thus, we shall think that the tensor of tension-shearing strain in the tangential plane is equal to zero:

$$\underline{\underline{\varepsilon}} = 0. \tag{2}$$

We have here ${}^4\underline{\underline{A}} \to \infty$, the corresponding relation of elasticity loses its meaning, and the force tensor in the tangential plane $\underline{\underline{T}} \cdot \underline{\underline{a}}$ is determined directly from the dynamic equations. The tensor of rigidity in bending and torsion ${}^4\underline{\underline{C}}$ has the form

$${}^4\underline{\underline{C}} = D\left[\frac{1+\nu}{2}\underline{\underline{c}}\,\underline{\underline{c}} + \frac{1-\nu}{2}\left(\underline{\underline{a}}_2\underline{\underline{a}}_2 + \underline{\underline{a}}_4\underline{\underline{a}}_4\right)\right]. \tag{3}$$

Here, D is the flexural rigidity of the shell, $\underline{\underline{a}}_2 = \underline{e}_{\varphi}\underline{e}_{\varphi} - \underline{e}_z\underline{e}_z$, and $\underline{\underline{a}}_4 = \underline{e}_{\varphi}\underline{e}_z + \underline{e}_z\underline{e}_{\varphi}$.

Obviously, in the absence of tension-shearing deformation, all quantities characterizing the stress-strain state of the shell depend only on the polar angle θ. As the main variable, we choose the displacement along a normal to the shell surface w. Then the problem of natural vibrations of the shell is reduced to the solution of a differential equation

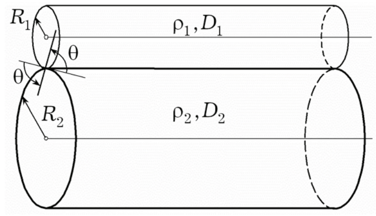

Fig. 1

$$\frac{D}{\rho R^4}\left(\frac{\partial^2}{\partial\theta^2}+1\right)^2\frac{\partial^2 w}{\partial\theta^2}+\left(\frac{\partial^2}{\partial\theta^2}-1\right)\frac{\partial^2 w}{\partial t^2} = 0\,. \tag{4}$$

The quantities characterizing the stress-strain state of our shell are connected with w by the relations

$$\frac{\partial u_\theta}{\partial\theta} = -w, \qquad \varphi_z = \frac{1}{R}\left(u_\theta-\frac{\partial w}{\partial\theta}\right), \qquad \frac{1}{R}\left(\frac{\partial^2 T_{\theta\theta}}{\partial\theta^2}+T_{\theta\theta}\right) = -2\rho\frac{\partial^2 w}{\partial t^2},$$

$$\frac{1}{R}\left(\frac{\partial T_{\theta r}}{\partial\theta}+\frac{\partial^3 T_{\theta r}}{\partial\theta^3}-1\right)^2 = \rho\left(\frac{\partial^2}{\partial\theta^2}-1\right)\frac{\partial^2 w}{\partial t^2}, \qquad M_{\theta z} = -\frac{D}{R^2}\left(\frac{\partial^2 w}{\partial\theta^2}+w\right). \tag{5}$$

The other components of vectors $\underline{u}$, $\underline{\varphi}$ and tensors $\underline{\underline{T}}$, $\underline{\underline{M}}$ are identically equal to zero.

Natural Vibrations of a System of Two Cylindrical Shells

Consider a system of two cylindrical shells of equal lengths but different radii. The shell of radius R_1, whose surface density and flexural rigidity are equal to ρ_1 and D_1, models the nanoobject under study. The shell of radius R_2, whose surface density and flexural rigidity are equal to ρ_2 and D_2, models the substrate, i.e., the microobject on which the nanoobject under study is situated. We assume that the axes of these cylinders are parallel, and they join between themselves along the line θ (see Fig. 1). The angle θ for each shell is counted off from the line of their joint anti-clockwise.

The kinematic conditions of junction of the shells look like

$$w^{(1)}\Big|_{\theta=0} = w^{(2)}\Big|_{\theta=0}, \qquad u_\theta^{(1)}\Big|_{\theta=0} = -u_\theta^{(2)}\Big|_{\theta=0}, \qquad \varphi_z^{(1)}\Big|_{\theta=0} = \varphi_z^{(2)}\Big|_{\theta=0}. \tag{6}$$

The force conditions of junction of the shells have the form

$$T_{\theta r}^{(1)}\Big|_{\theta=0} = T_{\theta r}^{(2)}\Big|_{\theta=0}, \qquad T_{\theta\theta}^{(1)}\Big|_{\theta=0} = -T_{\theta\theta}^{(2)}\Big|_{\theta=0}, \qquad M_{\theta z}^{(1)}\Big|_{\theta=0} = M_{\theta z}^{(2)}\Big|_{\theta=0}. \tag{7}$$

The conditions of closure of the shells can be formulated as

$$w^{(k)}\Big|_{\theta=0} = w^{(k)}\Big|_{\theta=2\pi}, \qquad u_\theta^{(k)}\Big|_{\theta=0} = u_\theta^{(k)}\Big|_{\theta=2\pi}, \qquad \varphi_z^{(k)}\Big|_{\theta=0} = \varphi_z^{(k)}\Big|_{\theta=2\pi}, \tag{8}$$

where $k = 1, 2$. The solutions of dynamic equations (4) for both shells have the following structure:

$$w^{(k)}(\theta, t) = W^{(k)}(\theta)e^{i\omega t}, \qquad W^{(k)} = \sum_{j=1}^{3}\Big[A_j^{(k)}\sin(\lambda_{kj}\theta) + B_j^{(k)}\cos(\lambda_{kj}\theta)\Big], \tag{9}$$

where ω is the natural frequency, $A_j^{(k)}$ and $B_j^{(k)}$ are arbitrary constants, and λ_{kj} are the roots of characteristic equations

$$\lambda_k^6 - 2\lambda_k^4 + (1-\Omega_k^2)\lambda_k^2 - \Omega_k^2 = 0, \qquad \Omega_k = \sqrt{\frac{\rho_k}{D_k}}R_k^2\omega. \tag{10}$$

Substituting expressions (9) and (10) in Eqs. (5), we can find all quantities characterizing the stress-strain state of the shells. Further, substituting the obtained solution in the boundary conditions (6)–(8), we obtain a homogeneous system of 12 algebraic equations in the constants $A_j^{(k)}$ and $B_j^{(k)}$. The condition of equality of the determinant of this system to zero gives the frequency equation. We choose the dimensionless frequency Ω_2 as the main variable. Then the coefficients of the frequency equation will depend on three dimensionless parameters R_1/R_2, ρ_1/ρ_2, and D_1/D_2. Hence, the solution of the frequency equation represents a spectrum of natural frequencies

$$\omega_n = \sqrt{\frac{D_2}{\rho_2}}\frac{\Omega_{2n}}{R_2^2}, \qquad \Omega_{2n} = \Omega_{2n}\left(\frac{R_1}{R_2}, \frac{\rho_1}{\rho_2}, \frac{D_1}{D_2}\right). \tag{11}$$

A Method for the Experimental Determination of the Flexural Rigidity of Nanoshells

Consider two systems of cylindrical shells with different physical and geometrical characteristics but with identical conditions of fastening (6)–(8) and equal dimensionless parameters

$$\frac{R_1}{R_2} = \frac{R_3}{R_4}, \qquad \frac{\rho_1}{\rho_2} = \frac{\rho_3}{\rho_4}, \qquad \frac{D_1}{D_2} = \frac{D_3}{D_4}. \tag{12}$$

The first system consists of nano- and microshell. The natural frequencies of this system are denoted by $\omega_n^{(1)}$. The second system consists of micro- and macroshell, and its natural frequencies are denoted by $\omega_n^{(2)}$. According to (11) and (12), the spectra of dimensionless natural frequencies of the systems under consideration coincide:

$$\Omega_{2n}^{(1)} = \Omega_{2n}^{(2)}, \tag{13}$$

and the true natural frequencies of these systems $\omega_n^{(1)}$ and $\omega_n^{(2)}$ are connected with their dimensionless frequencies $\Omega_{2n}^{(1)}$ and $\Omega_{2n}^{(2)}$ by

$$\omega_n^{(1)} = \sqrt{\frac{D_2}{\rho_2}}\frac{\Omega_{2n}^{(1)}}{R_2^2}, \qquad \omega_n^{(2)} = \sqrt{\frac{D_4}{\rho_4}}\frac{\Omega_{2n}^{(2)}}{R_4^2}. \tag{14}$$

As follows from (13) and (14), the ratio between the natural frequencies $\omega_n^{(1)}/\omega_n^{(2)}$ is independent of their ordinal number n:

$$\frac{\omega_n^{(1)}}{\omega_n^{(2)}} = \frac{R_4^2}{R_2^2}\sqrt{\frac{D_2\rho_4}{D_4\rho_2}}. \tag{15}$$

Thus, relations (12) and (15) can serve as a theoretical foundation for the experimental determination of the flexural rigidity of nanoshells. For determining flexural rigidity, it is necessary to carry out the following measurements and calculations:

(i) to measure several first natural frequencies of the system of nano- and microshell $\omega_n^{(1)}$;

(ii) to take, for comparison, the system of micro- and macroshell and, changing the parameters of this system and measuring its natural frequencies $\omega_n^{(2)}$, to achieve a situation where the ratios $\omega_n^{(1)}/\omega_n^{(2)}$ are independent of the ordinal number of frequencies n;

(iii) to find the flexural rigidities of micro- and macroshells and, using the last relation (12), to calculate the flexural rigidity of the nanoshell under consideration.

Asymptotic Estimates

The proposed method will be efficient if it is possible to realize it for a system where the sizes of the object under study are at least by an order of magnitude smaller than the substrate sizes. In order that this experiment should be practically realizable, the relative differences between natural frequencies of the system nanoobject-substrate $\omega_n^{(1)}$ and those for the substrate without the nanoobject $\omega_n^{(0)}$

$$\delta_n = \frac{\omega_n^{(1)} - \omega_n^{(0)}}{\omega_n^{(1)}} \tag{16}$$

have to be within the limits of accuracy of the measuring instrument. Let us evaluate the order of δ_n. Let $\omega_n^{(0)}$ be the natural vibration frequencies of a cylindrical shell with parameters R_2, ρ_2, and D_2, for which boundary conditions are formulated in the form of closure conditions (8) and conditions

$$T^{(2)}_{\theta r}\Big|_{\theta=0} = 0, \qquad T^{(2)}_{\theta\theta}\Big|_{\theta=0} = 0, \qquad T^{(2)}_{\theta r}\Big|_{\theta=0} = 0\,. \tag{17}$$

Obviously, the natural frequencies of the system of nano- and microshell $\omega_n^{(1)}$ will differ slightly from the natural frequencies of the microshell $\omega_n^{(0)}$. Hence, we may represent the frequencies $\omega_n^{(1)}$ as

$$\omega_n^{(1)} = \omega_n^{(0)} + \varepsilon\tilde{\omega}_n\,, \tag{18}$$

where ε is a dimensionless small parameter. Asymptotic analysis of system (5)–(10) shows that the introduced small parameter is equal to

$$\varepsilon = \frac{\rho_1 R_1^2}{\rho_2 R_2^2}\,. \tag{19}$$

Relations (16)–(19) enable us to evaluate the order of relative difference between the frequencies of the system nanoobject-substrate and frequencies of the substrate without the nanoobject: $\delta_n \sim \varepsilon$. The existing measuring technology makes it possible to measure natural frequencies with a relative error of $10^{-4}\%$. The δ_n value is at the limit of the resolution of measuring instruments if the linear sizes of nano- and microshell differ by 100 times.

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