An Approach to the Experimental Determination of the Bending Stiffness of Nanosize Shells

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The problem of the experimental determination of elastic moduli of nanoscale objects is of present interest. The determination of the elastic moduli of thin macroscopic shells is usually based on experiments with plates. It is known that, when grown using certain techniques, nanoobjects are obtained only in the form of shells. Therefore, it is necessary to develop a method for determining the elastic moduli of nanoobjects on the basis of experiments with shells. Experimental determination of the bending stiffness of nanosize shells presents a serious problem, because for such widespread nanoobjects as nanotubes and fullerenes under arbitrary deformation, the material is subjected to both bending and tension. Therefore, all parameters (e.g., natural frequencies) that can be measured directly are complicated functions of both bending and tension stiffness. In recent years, together with nanotubes and fullerenes, nanoobjects of a more intricate configuration have been obtained [1-4]. Nanosize cylindrical helices [1, 3] are of particular interest in connection with the possible experimental determination of bending stiffness. This is due to the fact that (1) in helical shells under arbitrary deformation, the material is mainly bent, so that the material tension effect can be neglected when interpreting experimental data; and (2) the natural oscillation shapes of helical shells are much more easily observed than those of cylindrical shells associated with pure bending of the material. The latter statement is illustrated in Fig. 1, which presents the first four helical shell oscillation shapes. The analysis of helical shell dynamics [5] presented below may be a theoretical foundation for experimental testing of the applicability of the continuum theory to (a) the calculation of mechanical characteristics of nanoobjects and (b) the experimental determination of the bending stiffness of nanoshells.

BASIC EQUATIONS OF THIN SHELL THEORY

We present here a summary of basic equations from the classical linear theory of shells. For the sake of brevity, we use the apparatus of direct tensor calculus [6, 7]. The dynamic equations have the form

$$\nabla \cdot \underline{\underline{T}} = \rho \underline{\underline{u}}, \quad \nabla \cdot \underline{\underline{M}} + \underline{\underline{T}}_{\times} = 0, \tag{1}$$

where $\underline{\underline{T}}$ and $\underline{\underline{M}}$ are the force and momentum tensors, respectively; ()_× is the vector invariant of a tensor; ρ is the surface mass density; and $\underline{\underline{u}}$ is the displacement vector. In the classical theory of shells, the transverse shear strain vector is assumed to be zero. Thus, the angle-ofrotation vector $\underline{\phi}$ can be expressed in terms of the displacement vector as

$$\varphi = -\underline{n} \times (\nabla \underline{u}) \cdot \underline{n}, \qquad (2)$$

where <u>n</u> is the unit normal vector to the shell surface. The transverse force vector $\underline{N} \equiv \underline{\underline{T}} \cdot \underline{\underline{n}}$ is determined from dynamic equations (1). The elasticity equation for the force tensor in the tangent plane $\underline{\underline{T}} \cdot \underline{\underline{a}}$ has the form

$$\underline{\underline{T}} \cdot \underline{\underline{a}} + \frac{1}{2} (\underline{\underline{M}} \cdot \cdot \underline{\underline{b}}) \underline{\underline{c}} = {}^{4} \underline{\underline{A}} \cdot \cdot \underline{\underline{\varepsilon}}.$$
(3)

The elasticity equation for the momentum tensor \underline{M}



Fig. 1. Oscillation shapes of a helical cylindrical shell.

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The dimensionless coordinates *s* and ζ vary within the following limits

$$-\frac{l}{2} \le Rs \le \frac{l}{2}, \quad -\frac{a}{2} \le R\zeta \le \frac{a}{2}.$$
 (7)

The unit vectors \underline{e}_s and \underline{e}_{ζ} directed along the coordinate lines and the unit vector \underline{n} determining the direction of the outward normal to the shell surface have the form

$$\underline{e}_{s} = \cos\alpha \underline{e}_{\varphi} + \sin\alpha \underline{k},$$

= $-\sin\alpha \underline{e}_{\varphi} + \cos\alpha \underline{k}, \quad \underline{n} = \underline{e}_{r}.$ (8)

APPROXIMATE EQUATIONS GOVERNING THE DYNAMICS OF A THIN HELICAL SHELL

It is known that the tensor ${}^{4}\underline{A}$ of the tension-shear stiffness of the shell in the tangent plane is proportional to the shell thickness h, while the tensor ${}^{4}\underline{C}$ of the bend-ing-torsion stiffness is proportional to h^{3} . Therefore, in the case $\frac{h}{a} \ll 1$ and $\frac{h}{l} \ll 1$, the helical shell under consideration can be treated as inextensible. Thus, we will assume that the tension-shear strain tensor in the tangent plane is equal to zero

$$\underline{\varepsilon} = 0. \tag{9}$$

In this case ${}^{4}\underline{A} \to \infty$, elasticity equation (3) becomes meaningless, and the force tensor in the tangent plane $\underline{T} \cdot \underline{a}$ is determined from dynamic equations (1) with regard to the strain compatibility equation

$$\Delta(\operatorname{tr}(\underline{T} \cdot \underline{a})) - (1 + \nu)\nabla \cdot (\nabla \cdot (\underline{T} \cdot \underline{a})) = 0, \quad (10)$$

where v is the Poisson's ratio. We note that the continuity equation (10) follows from the assumption that the tension-shear strain is absent in the tangent plane. Thus, the problem is reduced to the solution of the system of equations (1), (2), (4), (5), (9), and (10), where the bending-torsion stiffness tensor ${}^{4}\underline{C}$ has the form

$${}^{4}\underline{\underline{C}} = D\left[\frac{1+\nu}{2}\underline{\underline{c}}\underline{\underline{c}} + \frac{1-\nu}{2}(\underline{\underline{a}}_{2}\underline{\underline{a}}_{2} + \underline{\underline{a}}_{4}\underline{\underline{a}}_{4})\right].$$
(11)

Here *D* is the bending stiffness of the shell, $\underline{a}_2 = \underline{e}_s \underline{e}_s - \underline{e}_{\zeta} \underline{e}_{\zeta}$, and $\underline{a}_4 = \underline{e}_s \underline{e}_{\zeta} + \underline{e}_{\zeta} \underline{e}_s$.

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Fig. 2. Helical cylindrical shell.

has the form

$$\underline{\underline{M}}^{T} = {}^{4}\underline{\underline{C}} \cdot \cdot \underline{\underline{\kappa}}.$$
⁽⁴⁾

Here ${}^{4}\underline{A}$ and ${}^{4}\underline{C}$ are the shell stiffness tensors, \underline{a} is the unit tensor in the tangent plane, $\underline{b} = -\nabla \underline{n}, \ \underline{c} = -\underline{a} \times \underline{n}$, and the tension-shear strain tensor $\underline{\varepsilon}$ in the tangent plane and the bending-torsion strain tensor $\underline{\kappa}$ are calculated by the formulas

$$\underline{\underline{\varepsilon}} = \frac{1}{2} ((\nabla \underline{u}) \cdot \underline{\underline{a}} + \underline{\underline{a}} \cdot (\nabla \underline{u})^T),$$

$$\underline{\underline{\varepsilon}} = (\nabla \underline{\phi}) \cdot \underline{\underline{a}} + \frac{1}{2} ((\nabla \underline{u}) \cdot \cdot \underline{\underline{c}}) \underline{\underline{b}}.$$
(5)

HELICAL SHELL GEOMETRY

We will consider a cylindrical helical shell (Fig. 2) of radius *R* with helix angle α , helix-forming band length *l*, band width *a*, and band thickness *h*. Shell kinematics will be described below using two coordinate systems: a cylindrical coordinate system $r \equiv R$, φ , *z*, where the *z* axis is directed along the helix axis; and a curvilinear coordinate system *s*, ζ introduced on the shell surface as follows:

$$z = R(\sin\alpha s + \cos\alpha\zeta), \quad \varphi = \cos\alpha s - \sin\alpha\zeta.$$
 (6)

SOLUTION OF THE DYNAMIC EQUATIONS FOR A THIN HELICAL SHELL

The displacement vector is represented in the form of the decomposition in the $\underline{u} = u_s \underline{e}_s + u_{\zeta} \underline{e}_{\zeta} + w\underline{n}$ basis. The displacement w along the normal to the shell surface is chosen as the main variable. Using rather simple transformations, we reduce the equations of shell motion to the single differential equation

$$\left(\sin^2 \alpha \frac{\partial^4}{\partial s^4} + \cos^2 \alpha \frac{\partial^4}{\partial \zeta^4} - \frac{1}{4} \frac{\partial^4}{\partial s^2 \partial \zeta^2} \right)$$

$$\times \left[\frac{D}{\rho R^4} (\tilde{\Delta} + 1)^2 w + \ddot{w} \right] - \frac{\sin^2 2\alpha}{4} \tilde{\Delta} \ddot{w} = 0,$$

$$(12)$$

where $\tilde{\Delta} \equiv R^2 \Delta$ is the dimensionless Laplace operator. Representing condition (9) of the absence of tension– shear strain from the tangent plane in the coordinate form, we obtain the following relationship between the displacement vector components:

$$\frac{\partial u_s}{\partial s} = -\cos^2 \alpha w, \quad \frac{\partial u_\zeta}{\partial \zeta} = -\sin^2 \alpha w,$$

$$\frac{\partial u_\zeta}{\partial s} + \frac{\partial u_s}{\partial \zeta} = \sin 2\alpha w$$
(13)

and arrive at the following the strain compatibility equation in displacements:

$$\sin 2\alpha \frac{\partial^2 w}{\partial s \partial \zeta} + \sin^2 \alpha \frac{\partial^2 w}{\partial s^2} + \cos^2 \alpha \frac{\partial^2 w}{\partial \zeta^2} = 0.$$
(14)

We note that Eq. (14) is a direct consequence of Eqs. (13).

Thus, the problem is reduced to the determination of solutions of dynamic equations (12) that satisfy an additional constraint imposed by strain compatibility equation (14). In the cylindrical coordinates [see Eqs. (6)], strain compatibility equation (14) takes the form

$$\frac{\partial^2 w}{\partial z^2} = 0. \tag{15}$$

The solutions of dynamic equation (12) that satisfy strain compatibility equation (15) can obviously be represented as

$$w(\varphi, z, t) = W(\varphi, z)e^{i\omega t},$$

$$W(\varphi, z) = zW_1(\varphi) + W_2(\varphi).$$
(16)

Substituting expressions (16) into dynamic equation (12) and equating the coefficients of different powers of z to zero, we obtain the system of two differential equations

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in the variables $W_1(\varphi)$ and $W_2(\varphi)$. Solving this system and returning to the variables *s* and ζ , we obtain

$$W(s, \zeta) = \sum_{j=1}^{3} [(A_{j}^{s}(p_{j}s + q_{j}\zeta) + B_{j}^{s})]$$

$$\times \sin[\lambda_j(\cos\alpha s - \sin\alpha\zeta)] + (A_j^c(p_j s + q_j\zeta) + B_j^c)$$

$$\times \cos[\lambda_j(\cos\alpha s - \sin\alpha\zeta)]], \qquad (17)$$

$$p_{j} = \sin \alpha - \beta_{j}, \quad q_{j} = \cos \alpha + \beta_{j},$$
$$\beta_{j} = \frac{2\cos 2\alpha \Omega^{2}}{9\cos \alpha (\lambda_{j}^{4} + (\Omega^{2} - 1)\lambda_{j}^{2} + 2\Omega^{2})},$$

where A_j^s , B_j^s , A_j^c , and B_j^c are arbitrary constants and λ_i are the roots of the characteristic equation

$$\lambda^{6} - 2\lambda^{4} + (1 - \Omega^{2})\lambda^{2} - \frac{4}{3}\Omega^{2} = 0, \ \Omega = \sqrt{\frac{\rho R^{4}}{D}}\omega.$$
 (18)

Here, Ω is the dimensionless natural frequency; for its determination, some boundary conditions should be formulated. As follows from Eqs. (17) and (18), the dimensionless frequency Ω is independent of the physical characteristics of the shell ρ and *D* if these parameters do not enter into the boundary conditions.

FORMULATION OF THE BOUNDARY CONDITIONS. DETERMINATION OF THE NATURAL FREQUENCIES OF OSCILLATIONS OF A THIN HELICAL SHELL

In accordance with Eq. (17), the function $W(s, \zeta)$ involves twelve constants, which, naturally, make it impossible to satisfy all the boundary conditions of the classical theory of shells. However, the formulation of twelve homogeneous equations specifying the displacements or stresses at any point of the boundary is sufficient for a formal solution of the problem within the framework of the simplified formulation under consideration.

We will assume that the shell is fixed at corners; i.e., the displacement vector $\underline{u}(s, \zeta, t) = \underline{u}_*(s, \zeta)e^{i\omega t}$ is zero at the corner points

$$\underline{u}_*\left(\frac{l}{2R}, \frac{a}{2R}\right) = 0, \quad \underline{u}_*\left(-\frac{l}{2R}, \frac{a}{2R}\right) = 0,$$

$$\underline{u}_*\left(\frac{l}{2R}, -\frac{a}{2R}\right) = 0, \quad \underline{u}_*\left(-\frac{l}{2R}, -\frac{a}{2R}\right) = 0.$$
(19)

From the condition that the determinant of system (19) is equal to zero, we obtain the frequency equation. As

can be seen from Eqs. (13) and (15)-(18), the determinant of system (19) depends on the dimensionless fre-

quency Ω and three dimensionless parameters α , $\frac{l}{R}$,

and $\frac{a}{R}$. Therefore, the solution of the frequency equation represents a spectrum of dimensionless natural fre-

quencies of the form

$$\Omega_n = \Omega_n \left(\alpha, \frac{l}{R}, \frac{a}{R} \right), \quad n = 1, 2, \dots$$
 (20)

Numerical calculations of the natural frequencies and shapes of helical shell oscillations with the dimensionless parameters $\alpha = \frac{\pi}{6}$, $\frac{l}{R} = 20\pi$, and $\frac{a}{R} = 1$ showed that the approximate theory specified by Eqs. (17)–(19) adequately describes low-frequency oscillations.

DISCUSSION OF THE RESULTS

We will consider two thin helical shells with different physical and geometric characteristics but the same dimensionless parameters α , $\frac{l}{R}$, and $\frac{a}{R}$. We will assume that both shells are fixed at corners; i.e., boundary conditions (19) apply. In this case, in accordance with Eq. (20), the spectra of the dimensionless natural frequencies of shells under consideration coincide with

$$\forall n: \ \Omega_n^{(1)} = \Omega_n^{(2)}.$$
 (21)

Then, in accordance with Eq. (18), the natural frequency ratio $\frac{\omega_n^{(1)}}{\omega^{(2)}}$ is independent of their ordinal num-

ber n

$$\frac{\omega_n^{(1)}}{\omega_n^{(2)}} = \sqrt{\frac{D_2 \rho_1 R_1^4}{D_1 \rho_2 R_2^4}}.$$
 (22)

Relation (22) may serve as a theoretical basis for the experimental investigation of the applicability of the continuum theory to nanoobjects and, if the answer is affirmative, for experimental determination of the bending stiffness of nanoshells.

EXPERIMENTAL TESTING OF THE APPLICABILITY OF THE CONTINUUM THEORY TO NANOSCALE OBJECTS

To test the applicability of the continuum theory to nanoobjects, the following measurements can be performed: (1) several first natural frequencies of a helical nanoshell are measured;

(2) the natural frequencies of a macroscopic helical shell with the same dimensionless parameters α , $\frac{l}{R}$,

and $\frac{a}{R}$ and the same fixation conditions are measured;

(3) the measured frequency ratios
$$\delta_n = \frac{\omega_n^{(1)}}{\omega_n^{(2)}}$$
 are cal-

culated.

roscopic helical shells.

If the continuum theory is applicable to nanoobjects, then the equality $\delta_n = \delta_1$ theoretically holds true for any *n*. The applicability condition for the continuum theory is really formulated as the inequality $\frac{|\delta_n - \delta_1|}{\delta_1} \le \varepsilon_N$, which must be fulfilled for $\forall n \le N$. The permissible error ε_N can be estimated by comparing with the results of an analogous experiment performed with two mac-

EXPERIMENTAL DETERMINATION OF THE BENDING STIFFNESS OF NANOSHELLS

If the continuum theory is applicable to nanoobjects, then formula (22) makes it possible to experimentally determine the bending stiffness of a nanoshell. In order to determine the bending stiffness, it is necessary:

(1) to measure the first natural frequency $\omega_1^{(1)}$ of the helical nanoshell;

(2) to measure the mass m_1 and the geometric dimensions l_1 , a_1 , and R_1 of the nanoshell and to calcu-

late its surface density
$$\rho_1 = \frac{m_1}{l_1 a_1}$$
;

(3) to determine the characteristics $\omega_1^{(2)}$, D_2 , ρ_2 , and R_2 of a compared macroscopic helical shell with the same dimensionless parameters α , $\frac{l}{R}$, and $\frac{a}{R}$ and the same fixation conditions as those of the nanoshell under study;

(4) to calculate the bending stiffness of the nanoshell D_1 using formula (22).

We note that the proposed approach to the experimental determination of bending stiffness does not require the determination of nanoshell thickness [8, 9].

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