The Solid Mechanics and Nanotechnology

E. Ivanova[1], A.Krivtsov[1], N. Morozov[2], B. Semenov[2]
[1] Dep. of Teoretical Mechanics, St.-Petersburg State Polytechnical University,
Politechnicheskaya str., 29, St.-Petersburg, Russia, 195251.
[2] Dep. of Elasticity theory, St.-Petersburg State University,
Bibliotechnaya sq., 2, Staryi Petergof, St.-Petersburg, Russia, 198904.
morozov@NM1016.spb.edu

In recent years, rapid development of nanotechnologies led to the necessity of constructing adequate physical models that make it possible to describe physico-mechanical properties of objects with a nanometer-size (nanosize) scale. The majority of existing models of such a kind adopt that basic mechanical characteristics of nanosize objects correspond to those obtained in macroscopic experiments. However, when dealing with structures containing only several atomic layers, the discrepancy arises between the evident discreteness of an object under study and a continual method of its description. The inconsistency of values of elastic moduli, which were obtained in microscale and macroscale experiments, was noted by many researchers. The solution to an equivalent continual problem allows the Poisson's ratio and Young modulus for the coating to be determined from such experiments. However, the values of elastic characteristics measured by this method exhibit a substantial inconsistency by their macroscopic values for the same material. The aim of the presented paper is devoted to theoretical and experimental investigation of the influence of the scale effect for the Poisson's ratio, Young modulus and the bending stiffness of thin nanocrystalline structures. The interest to these problems is connected with the necessity of investigation of the mechanical deformation of nanotube devices, which are used intensively in the recent years in nanotechnology developments. Engineering materials and structures at the nanoscale are expected to play a key role in the production of the next generation of electronic devices such as single electron transistors, terabit memories, quantum computers, and etc.

Poisson's ratio and Young modulus determination. We consider a two-dimensional single crystal shown in the Fig. 1. The crystal possesses an infinite length along the x direction and $N > 2$ atomic layers in the direction. Each

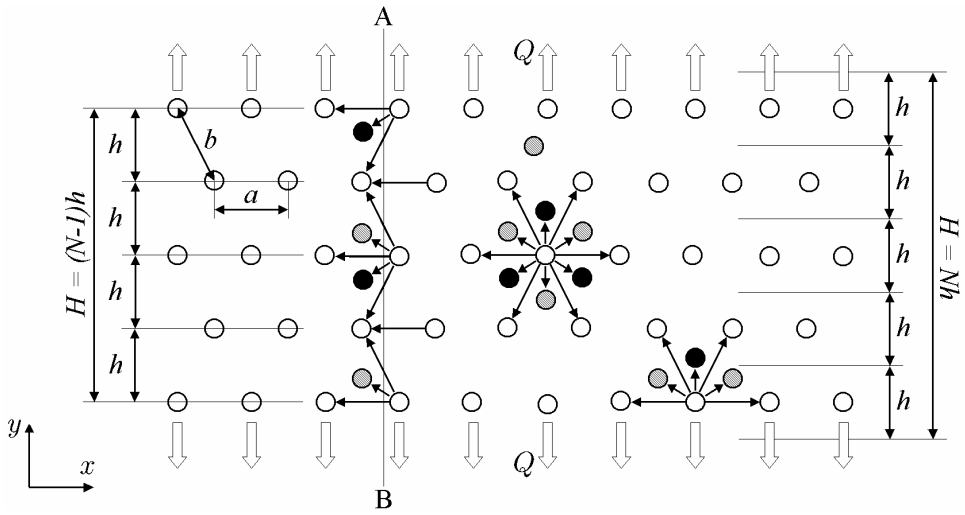

FIGURE 1.

atom interacts only with its nearest neighbors, as is shown in the Fig. 1. Constant tensile forces Q are applied to atoms located at crystal ends. The deformed single-crystal state under consideration is completely determined by the distance a between neighboring atoms in each layer and by the interlayer distance h. Let us note, that the crystal thickness H (its extension along the y direction), in principle, cannot be determined unambiguously. For example, if we assume that the crystal thickness is equal to the distance between atomic layers lying on opposite crystal ends (see Fig. 1), then, in this case, $H = (N-1)h$. On the other hand, it is quite reasonable to determine the crystal thickness as a product of the number of layers by the thickness of a single layer, which results in the formula $H = Nh$. Therefore, we denote $H = N_* h$, $N - 1 \le N_* \le N$, where N_* is the quantity reflecting an arbitrariness in the determination of H. The crystal under consideration is anisotropic. We recall that the infinite crystal with the HCP crystal lattice is isotropic and, hence, the anisotropy indicated is a manifestation of the scale factor. urthermore, we denote

$$\nu_1 = -\left.\frac{\varepsilon_2}{\varepsilon_1}\right|_{\sigma_2=0}, \qquad E_1 = \left.\frac{\sigma_1}{\varepsilon_1}\right|_{\sigma_2=0}, \qquad \nu_2 = -\left.\frac{\varepsilon_1}{\varepsilon_2}\right|_{\sigma_1=0}, \qquad E_2 = \left.\frac{\sigma_2}{\varepsilon_2}\right|_{\sigma_1=0}. \tag{1}$$

Here, ν_1 and E_1 are the Poisson's ratio and Young modulus for tension along the x axis; the quantities ν_2 and E_2 correspond to tension along the y axis. Using relationships (1) and equations of equilibrium of the crystal, we obtain [1]

$$\nu_1 = \nu_\infty, \qquad E_1 = \frac{N}{N_*} E_\infty, \qquad \nu_2 = \frac{N-1}{N-1/9}\nu_\infty, \qquad E_2 = \frac{N}{N-1/9} E_\infty, \tag{2}$$

where, ν_∞ and E_∞ are values of the Poisson's ratio and Young modulus, which correspond to the infinite crystal. Dependence of the Poisson's ratio and Young modulus on number of atomic layers is shown at Fig. 2.

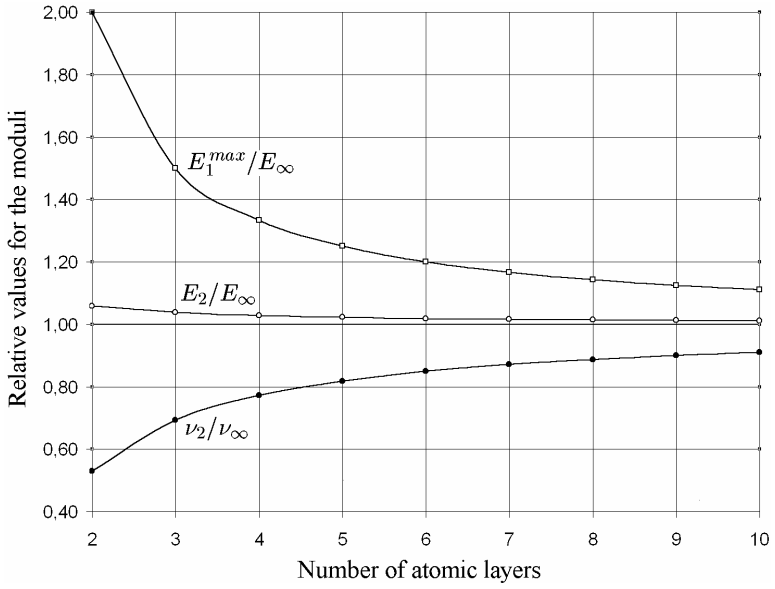

FIGURE 2.

Based on the studies performed, we can list the basic properties intrinsic to nanocrystals. 1. For the elastic moduli of a nanocrystal, only a possible interval of values is determined. This is associated with the impossibility of unambiguously determining the size of a nanoobject. 2. Elastic properties of a nanocrystal substantially depend on the number of atomic layers forming it. 3. The shape and size of a nanocrystal introduce an additional anisotropy into its elastic properties.

Bending stiffness determination. Let us consider a two-dimensional single crystal shown in Fig. 3. The crystal possesses $N \geq 1$ atomic layers in the y direction and $J >> N$ layers in the x direction. Forces Q_n are applied to atoms located at crystal end-walls, where n is the number of the horizontal layer, containing

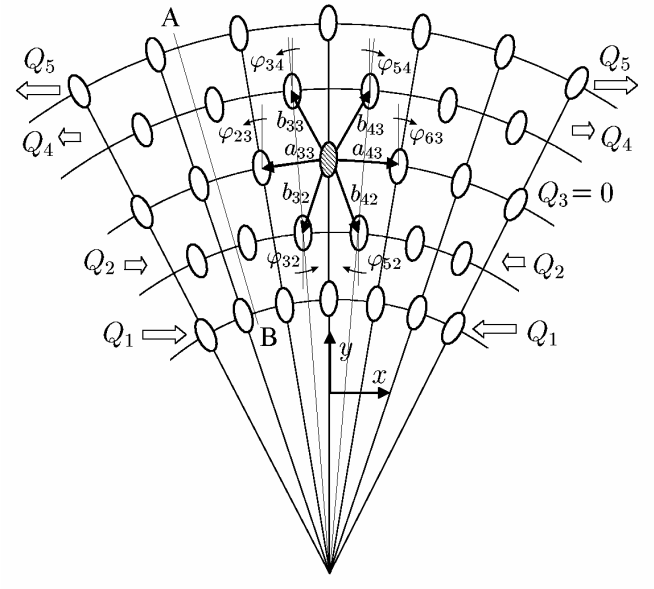

FIGURE 3.

the specified atom. These forces are changing linearly with coordinate, keeping the zero average value of the overall force acting on the end-wall, so that we can consider the macroscopic boundary conditions as an action of a pure moment (without tensile stress). If the moment interaction of particles is not taken into account, the bending stiffness of the monocrystal has the form [2]

$$D = D_\infty \left(1 - \frac{1}{N^2}\right), \qquad D_\infty = \frac{E_\infty H^3}{12}. \tag{3}$$

Here D_∞ is the value for the bending stiffness from the macroscopic theory of elasticity. According to formula (3), the bending stiffness of the nanocrystal is varying in the limits of $0 \leq D \leq D_\infty$. For the small values of N formula (3) gives the bending stiffness values smaller then D_∞ and finally it vanishes for $N = 1$. However, it is known that the bending stiffness of single-wall nanotubes does not equal to zero. Taking into account the moment interaction of particles, we obtain the following expression for the bending stiffness [3]

$$D = D_\infty \left(1 - \frac{1}{N^2}\right) + E_\infty^* \left(1 - \frac{1}{3N}\right), \tag{4}$$

where, E_∞ is the value of rotational Young modulus from the macroscopic moment theory of elasticity. It is easy to see that the bending stiffness of the nanocrystal given by formula (4) does not vanishe for $N = 1$.

Experimental method of determination of bending stiffness of nanoshells. 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 [4–6]. Nanosize cylindrical helices [4] (see Fig. 4) are of particular interest in connection with the possible experimental determination of bending stiffness.

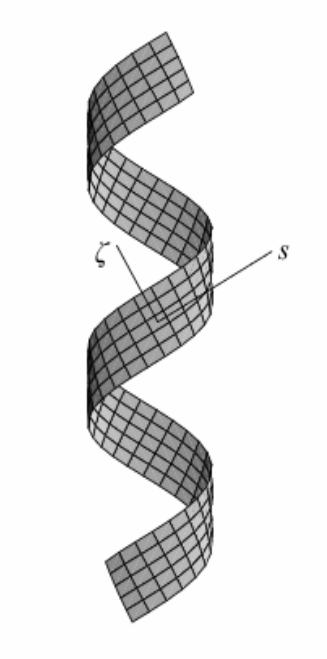

FIGURE 4.

This is due to the fact that 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 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. 5, which presents the first four helical shell oscillation shapes. The analysis of helical shell dynamics 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 [7].

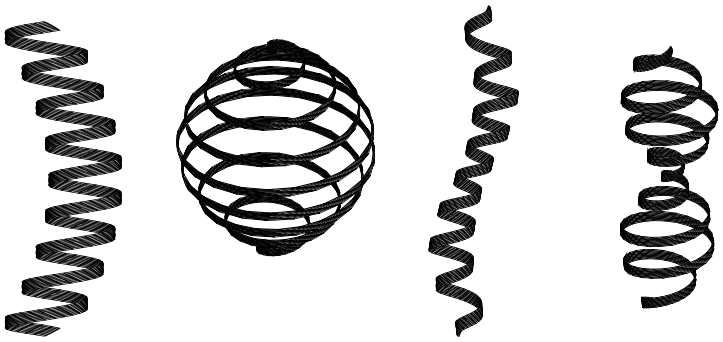

FIGURE 5.

Let us take into consideration dimensionless frequency

$$\Omega = \sqrt{\frac{\rho R^4}{D}}\omega, \tag{5}$$

where, ρ is the surface mass density, R is radius of cylindrical helical shell, D is ending stiffness, and ω is eigenfrequency. It is shown, that dimensionless frequencies Ω_n depend on the number of frequency n and three dimensionless parameters

$$\Omega_n = \Omega_n\left(\alpha, \frac{l}{R}, \frac{a}{R}\right), \tag{6}$$

where, α is helix angle, l is helix-forming band length, a is helix-forming band width.

We will consider two thin helical shells with different physical and geometric characteristics but the same dimensionless parameters α, l/R, and a/R. We will assume that both shells are fixed at corners. In this case, the spectra of the dimensionless frequencies of shells under consideration coincide with (6). Then, in accordance with (5), the frequency ratio $\omega_n^{(1)}/\omega_n^{(2)}$ is independent of their ordinal number n

$$\frac{\omega_n^{(1)}}{\omega_n^{(2)}} = \sqrt{\frac{D_1\rho_2 R_2^4}{D_2\rho_1 R_1^4}}. \tag{7}$$

Relation (7) 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.

To test the applicability of the continuum theory to nanoobjects, the following measurements can be performed: 1) Several first eigenfrequencies of a helical nanoshell are measured. 2) The eigenfrequencies of a macroscopic helical shell with the same dimensionless parameters α, l/R, a/R, and the same fixation conditions are measured. 3) The measured frequency ratios $\delta_n = \omega_n^{(1)}/\omega_n^{(2)}$ are calculated. 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 macroscopic helical shells.

If the continuum theory is applicable to nanoobjects, then formula (7) 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 eigenfrequency $\omega_1^{(1)}$ 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 calculate 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, l/R, 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 (7).

Methods of measuring of eigenfrequencies. Acoustical and optical methods of measuring of the eigenfrequencies of micro-objects are based on using homodyne laser vibrometers and adaptive photodetectors. Technique for vibration analysis of the laser vibrometer using adaptive photodetectors is based on the effect of non-steady-state photoelectromotive force. The technique enables efficient direct conversion of high-frequency phase modulation of speckle-like optical waves reflected from the vibrating object into output electrical signal with concomitant setting of the optimal operation point of the interferometer and suppression of amplitude laser noise. Methods of measuring of the eigenfrequencies of nano-objects are based on using atomic force microscope. Technique for vibration analysis is based on the effect of mechanical interaction of cantilever needle with nano-object.

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