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MECHANICS

On the Determination of Rigidity Parameters for Nanoobjects

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The goal of the present study is to develop theoretical principles for experimentally determining the rigidity parameters of nanometer-size objects (nanoobjects). It is well known that one of the most efficient methods for the determination of elastic moduli used in macroscopic mechanics is based on measurements of the eigenfrequencies of objects under investigation. In this paper, we discuss subtle features arising when such a method is applied in studying nanoobjects. We propose a method for experimentally determining their rigidity parameters, which is based on the phenomenon of the dynamical quenching of so-called "antiresonance" vibrations. The advantage of this method is the possibility to isolate eigenfrequencies of a nanoobject under study from the entire spectrum of a nanoobject–cantilever system of an atomic-force microscope (AFM).

Recently, the problem of the determination of elastic moduli intrinsic to nanoobjects has become urgent. In a number of studies, contradictions were noted between the values of elastic moduli obtained in experiments performed at the microscopic and macroscopic levels. In [1, 2], as an example, the dependences of both the Young modulus and the bending rigidities of samples were theoretically investigated for a two-dimensional single-crystal bar as functions of the number of atomic layers. Comparison of the results obtained in [1] and [2] shows that three expressions derived for the flexural rigidity of a rod differ significantly from each other. We mean the expression well known in continual theory; the expression obtained by the substitution of the Young modulus (calculated from the discrete model of [1]) into the formula for continual theory; and the expression directly obtained in the discrete model of [2] for the case of a small number of atomic layers. Thus, the development of methods for the direct determination of elastic properties of thin-walled nanoobjects (without using any formulas that associate elastic moduli of a nanoobject with its thickness and the Young modulus of the material) is a rather important problem. In particular, an urgent task is the experimental determination of mechanical characteristics of nanoobjects [3]. One of the most efficient methods for the determination of the elastic-modulus, which are employed in macroscopic mechanics, is based on measuring the eigenfrequencies of an object under study. Below, we discuss subtle features arising while using this (resonance) method as applied to nanoobjects. We also propose a new method based on antiresonance phenomenon.

At present, investigation of the properties of nanoobjects, including measuring their eigenvalues, is performed by probe-microscopy methods; in particular, AFM methods are used widely [4, 5]. The most important component of an atomic-force microscope is the scanning probe (cantilever) [6, 7]. Nowadays, standard industrial cantilevers have dimensions close to $200 \times 35 \times 1.5$ μm and resonance frequencies on the order of 10–400 kHz. In this case, the needle curvature radius can vary within the limits of 10–50 nm. However, there is a basic obstacle arising in the course of frequency measurements for an object under study by AFM methods, which is well known in mechanics. We imply the redistribution of vibration eigenfrequencies of the system (composed of a cantilever and a nanoobject to be studied) between eigenfrequencies of these objects taken separately [8]. In this case, the character of the spectral shift depends significantly on the distance between the needle point and the surface.

The statements made above indicate the fundamental differences between conditions in which experiments with nanoobjects and those with macroscopic objects are carried out. For the latter objects, the size of

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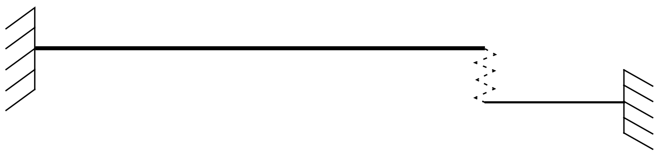

Fig. 1. Cantilever (at the left) and nanosize rod (at the right).

measuring devices (e.g., strain gauges) is considerably smaller than the dimensions of the object to be studied. While investigating nanoobjects, microscopic-sized equipment is employed. Therefore, the problem of investigating the interaction of nanoobjects with the measuring equipment becomes urgent. Below, this problem is discussed as applied to the experimental determination of elastic characteristics for nanoobjects by AFM methods. In fact, two tasks arise that lie at the boundary of mechanics and experimental physics.

The first task is the determination of nanoobject elastic moduli on the basis of the frequencies for a system composed of a nanoobject and the cantilever. The second task consists in providing experimental conditions for the isolation of nanoobject eigenfrequencies in the spectrum of the nanoobject–cantilever system.

The present paper is a natural continuation of study [6]. Here, we formulate the problem and describe a system formed by a cantilever and a nanoobject to be investigated. The basic difference is the fact that we deal with a nanoobject having its own dynamics. Components of thin-walled nanostructures such as rods, shells, and spirals can be considered as an adequate mechanical model. The theoretical substantiation of determining eigenfrequencies is developed by the AFM method for rod structures.

We now analyze the following mechanical model for an object under study (Fig. 1). The rod shown at the left models a cantilever. The left end of the rod is fixed, whereas the right end interacts with the object under investigation. The vertical deflection of the cantilever is described by the function $u(x_1, t)$, where x_1 is the coordinate along the rod, with the value $x_1 = 0$ corresponding to the cantilever left end. The following notation is used: L_1 is the cantilever length, and D_1 and ρ_1 are the flexural rigidity and the linear density, respectively. The rod shown at the right models an object being investigated for which it is necessary to find the flexural rigidity [9, 10]. The right end of the rod is rigidly fixed. The left end interacts with the cantilever. The vertical deflection of the rod is determined by the function $v(x_2, t)$, where x_2 is the coordinate along the rod, with the value $x_2 = 0$ corresponding to the nanosize-rod right end. The following notation is used: L_2 is the nanosize rod length, and D_2 and ρ_2 are the flexural rigidity and the linear density. The field interaction between the nanosize rod and the cantilever is modeled by the linear spring rigidity C that corresponds to the Leonard-Jones linearization potential (or any other interaction potential) in the region of the statically equilibrium state. In the truncated configuration, the rods and the spring are considered to be not deformed and not stressed, respectively.

The basic dynamical equations describing free vibrations of the mechanical system under study have the form

$$D_1 u^{\mathrm{IV}} + \rho_1 \ddot{u} = 0, \quad D_2 v^{\mathrm{IV}} + \rho_2 \ddot{v} = 0. \tag{1}$$

Equations (1) are supplemented by the necessary boundary conditions

$$\begin{gathered} u(0) = 0, \quad u'(0) = 0, \quad u''(L_1) = 0, \\ D_1 u'''(L_1) = C[u(L_1) - v(L_2)], \\ v(0) = 0, \quad v'(0) = 0, \quad v''(L_2) = 0, \\ D_2 v'''(L_2) = -C[u(L_1) - v(L_2)]. \end{gathered} \tag{2}$$

The spectral problem corresponding to Eqs. (1) and (2) is formulated for seeking eigenfrequencies of system vibrations; i.e., the solution is sought in the form

$$u(x_1, t) = u_0(x_1)e^{i\omega t}, \quad v(x_2, t) = v_0(x_2)e^{i\omega t}.$$

The solution of the formulated spectral problem is reduced to the following equations in terms of frequencies:

$$\begin{gathered} [1 + \cos(\lambda L_1)\cosh(\lambda L_1)](1 + \cos(\mu L_2)\cosh(\mu L_2) \\ + \frac{C}{D_2\mu^3}[\sin(\mu L_2)\cosh(\mu L_2) - \cos(\mu L_2)\sinh(\mu L_2)]) \\ + \frac{C}{D_1\lambda^3}[\sin(\lambda L_1)\cosh(\lambda L_1) - \cos(\lambda L_1)\sinh(\lambda L_1)] \\ \times(1 + \cos(\mu L_2)\cosh(\mu L_2)) = 0. \end{gathered} \tag{3}$$

Here, we have used the denotations

$$\lambda^2 = \sqrt{\frac{\rho_1}{D_1}}\omega, \quad \mu^2 = \sqrt{\frac{\rho_2}{D_2}}\omega,$$

where ω is the system eigenfrequency. As is seen from Eq. (3), all the eigenfrequencies are dependent on all the parameters of the system; therefore, it is impossible to isolate nanosize-rod frequencies in the system frequency spectrum. We now find the relation between the quantities $\frac{C}{D_1\lambda^3}$ and $\frac{C}{D_2\mu^3}$ using the known values for the flexural rigidities D_1 and D_2, as well as for wave numbers λ and μ. As a result, we arrive at the following inequality:

$$\frac{C}{D_1\lambda^3} \ll \frac{C}{D_2\mu^3}. \tag{4}$$

Thus, Eq. (3) expressed in terms of frequencies can be represented in the approximated form

$$[1 + \cos(\lambda L_1)\cosh(\lambda L_1)](1 + \cos(\mu L_2)\cosh(\mu L_2) + \frac{C}{D_2\mu^3}[\sin(\mu L_2)\cosh(\mu L_2) - \cos(\mu L_2)\sinh(\mu L_2)]) = 0 \quad (5)$$

Equation (5) has two spectra of eigenfrequencies. The first spectrum determines the vibration eigenfrequencies of the cantilever, namely,

$$1 + \cos(\lambda L_1)\cosh(\lambda L_1) = 0. \quad (6)$$

The second spectrum corresponds to the vibration eigenmodes of the nanosize rod with the spring-loaded end. This spectrum corresponds to the equation

$$1 + \cos(\mu L_2)\cosh(\mu L_2) + \frac{C}{D_2\mu^3}[\sin(\mu L_2)\cosh(\mu L_2) - \cos(\mu L_2)\sinh(\mu L_2)] = 0. \quad (7)$$

Thus, for not very strong assumption (4), the problem associated with the identification of the spectra for each of the objects is being solved because we managed to isolate the individual spectra. The natural problem is the determination of cantilever-vibration forms at the frequencies found above. This is rather important since they significantly affect the measurement quality in the case when the resonance is fixed by means of a laser beam with a spot of a finite diameter.

We consider stimulated harmonic vibrations of the system assuming that

$$u(0, t) = A\sin(\Omega t), \quad A = \text{const}. \quad (8)$$

The solution to the above-formulated problem is represented by the functions

$$\begin{aligned} u(x_1, t) &= [P_1\cos(\lambda_* x_1) + P_2\sin(\lambda_* x_1) \\ &+ P_3\cosh(\lambda_* x_1) + P_4\sinh(\lambda_* x_1)]\sin(\Omega t), \\ v(x_2, t) &= [Q_1\cos(\mu_* x_2) + Q_2\sin(\mu_* x_2) \\ &+ Q_3\cosh(\mu_* x_2) + Q_4\sinh(\mu_* x_2)]\sin(\Omega t), \end{aligned} \quad (9)$$

where $\lambda_*^2 = \sqrt{\frac{\rho_1}{D_1}}\Omega$ and $\mu_*^2 = \sqrt{\frac{\rho_2}{D_2}}\Omega$. The constant quantities P_i and Q_i are determined from the boundary conditions. Here, we do not write them out because they are too cumbersome. We should note that the denominators of the expressions for the constant quantities P_i and Q_i vanish when the stimulated-vibration frequency Ω coincides with one of the system eigenfrequencies ω_n determined by Eq. (3). In the framework of the model under consideration, for values $\Omega = \omega_n$, the vibration amplitude of the cantilever becomes infinitely large. In the real experiment, this amplitude rises steeply, which makes it possible to fix resonance frequencies coinciding with system eigenfrequencies.

We now analyze the effect of the dynamical damping of vibrations. Experimentally, one can fix not only the steep increase in the vibration amplitude but also its vanishing. In systems with distributed parameters, which are composed of several bodies, the vibration amplitude can vanish in two cases. In the first case, the point at which the amplitude is measured is a node of a given vibration form. In the second case, the dynamical damping of vibrations of one body occurs at the partial frequency of the other body. (This phenomenon is often called the "antiresonance".) We now pose the following question. Can exist frequencies Ω of stimulated vibrations for which the cantilever right end, being in contact with a nanosize object, would be immobile at an arbitrary instant of time? The answer can be found from the solution to the equation

$$u(L_1, t) = 0. \quad (10)$$

Substituting expression (9) for $u(x_1, t)$ into formula (10) and performing simple transformations with the expressions for the constant quantities P_i and Q_i taken into account, we arrive at the equation

$$\begin{aligned} &AD_1D_2\lambda_*^3\mu_*^3[2\cosh(\lambda_* L_1)\sin(\lambda_* L_1) \\ &+ 2\sinh(\lambda_* L_1)\cos(\lambda_* L_1) + \sinh(2\lambda_* L_1) \\ &+ \sin(2\lambda_* L_1)](1 + \cos(\mu_* L_2)\cosh(\mu_* L_2) \\ &+ \frac{C}{D_2\mu_*^3}[\sin(\mu_* L_2)\cosh(\mu_* L_2) \\ &- \cos(\mu_* L_2)\sinh(\mu_* L_2)]) = 0. \end{aligned} \quad (11)$$

Solving Eq. (11), we can determine the frequencies Ω_n for which the vibration amplitude of the cantilever right end vanishes. It is easy to understand that Eq. (11) is decomposed into two independent equations. The first

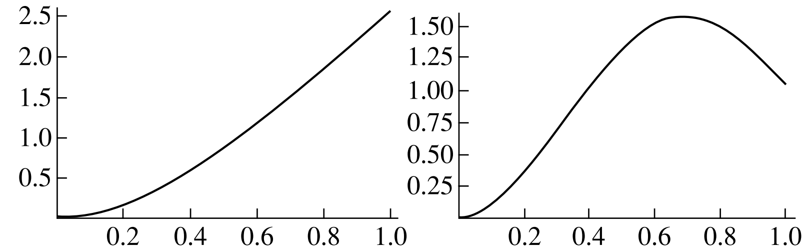

Fig. 2. Resonance forms ($\frac{L_2}{L_1}$ = 1.0, $\frac{h_2}{h_1}$ = 1.0). Here, as in Figs. 3 and 4, displacements of cantilever points and dimensionless coordinates x_1/L_1 are plotted along the vertical and horizontal axes, respectively.

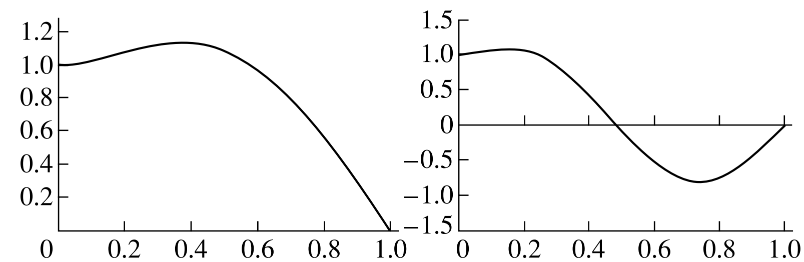

Fig. 3. Antiresonance forms ($\frac{L_2}{L_1}$ = 1.0, $\frac{h_2}{h_1}$ = 1.0).

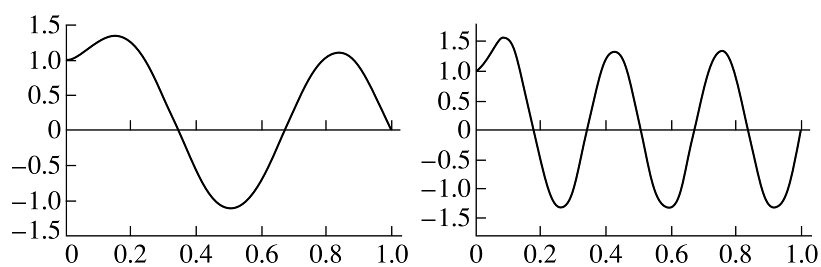

Fig. 4. Antiresonance forms ($\frac{L_2}{L_1}$ = 0.1, $\frac{h_2}{h_1}$ = 0.1).

of them is of the form

$$2\cosh(\lambda_* L_1)\sin(\lambda_* L_1) + 2\sinh(\lambda_* L_1)\cos(\lambda_* L_1) + \sinh(2\lambda_* L_1) + \sin(2\lambda_* L_1) = 0. \tag{12}$$

The second equation is written as

$$1 + \cos(\mu_* L_2)\cosh(\mu_* L_2) + \frac{C}{D_2\mu_*^3}[\sin(\mu_* L_2)\cosh(\mu_* L_2) - \cos(\mu_* L_2)\cosh(\mu_* L_2)] = 0. \tag{13}$$

Equation (12) depends on the cantilever parameters only and is of no interest. Equation (13) depends on the parameters of both the nanosize rod and the rigidity, as well as on the coupling rigidity between the rod and the cantilever. This is the equation that determines the antiresonance frequencies responsible for the dynamical quenching of the cantilever right-end vibrations. We should note that Eq. (13) exactly coincides with Eq. (7), which determines the eigenfrequencies of the spring-loaded nanosize rod. Insofar as Eq. (7) was obtained from the frequency equation (3) by neglecting small quantities on the order of $\frac{C}{D_1\lambda^3}$, we may state that the antiresonance frequencies Ω_n are close to the system eigenfrequencies ω_n and differ from them by small quantities of the indicated order of magnitude.

In Figs. 2–4, the first two forms of cantilever vibrations are presented for the resonance and antiresonance cases. The resonance vibration forms are shown in Fig. 2. (In this and the following figures, the vertical and horizontal coordinate axes correspond to the displacements of the cantilever points and the dimensionless coordinates $\frac{x_1}{L_1}$, respectively.) The plot corresponds to the case of identical sizes of the cantilever and the rod under investigation. While decreasing the rod size, the cantilever vibration forms do not qualitatively vary. Using the AFM method, we can fix the resonances sufficiently simply. The only significant disadvantage of the method is the fact that the resonance frequencies characterize not the object under study but the entire system including both this object and the cantilever. In this connection, it is extremely important to the existence of the antiresonance phenomenon, in so far as it allows us to determine the vibration eigenfrequencies of the nanostructure being studied. The cantilever vibration forms that correspond to the antiresonance frequencies are multimodal. The number of nodes is determined by both the ordering number of the form and the parameter

$$\sqrt[4]{\frac{D_1\rho_2}{D_2\rho_1}}\frac{L_2}{L_1} \sim \sqrt{\frac{h_1}{h_2}}\frac{L_2}{L_1},$$

where h_1 and h_2 are cross-section characteristic sizes for the cantilever and the rod being investigated, respectively. If their sizes are identical, the first antiresonance vibration form of the cantilever is free of nodes, whereas the second form has one node (Fig. 3). With a decrease in all linear sizes of the rod by a factor of 10, the values of the antiresonance frequencies increase by the same factor, whereas the first forms of the cantilever vibrations become multimodal (Fig. 4). The increase in the antiresonance frequencies can lead to the fact that they will turn out to be beyond the limits of the frequency region of the measuring devices. Attempts aimed at fixing the antiresonance according to the multimodal form can be accompanied by the appearance of unexpected problems. They are associated with the fact that the laser beam used by the optical registration system determining the deviation of the cantilever by the AFM method [11] is not a point but a spot of finite dimensions. Therefore, in the measurements, the average value of the amplitude in a rod segment rather than the amplitude at a certain rod point is determined. If the length of the rod under study decreases less significantly than the characteristic sizes of its cross section, then the values of the antiresonance frequencies and the number of nodes on the cantilever vibration forms increase less rapidly. Thus, for certain relations between the parameters of the cantilever and the object under study, the cantilever vibration forms make it possible to use existing laser devices in order to attain the antiresonance.

The question on the determination of rigidity characteristics of nanosize objects was also analyzed in [12]. In the present case, the flexural rigidity of the nanosize rod can be determined according to both the resonance and antiresonance frequencies [on the basis of Eqs. (3) and (13), respectively]. The equations contain two unknown parameters: the flexural rigidity D_2 of the nanosize rod and the rigidity C for the coupling of the cantilever needle with this rod. (The cantilever parameters are known; the nanosize-rod mass m_2 and length L_2 can be measured. The linear density for a homogeneous rod is calculated according to the formula $\rho_2 = \frac{m_2}{L_2}$. If two (resonance or antiresonance) frequencies are measured, their values can be substituted into corresponding equations (3) or (13). As a result, the problem of determining the flexural rigidity of a nanosize rod is reduced to solving the set of two transcendental equations with respect to two unknowns. It should be noted that Eq. (13) for the antiresonance frequencies is simpler than Eq. (3) and, in contrast to (3), does not contain the small parameter $\frac{C}{D_1\lambda^3}$. Thus, from the calculation standpoint, the method of the determination of the flexural rigidity for a nanosize rod according to its antiresonance frequencies has certain advantages. However, in order to improve the measurement reliability, it is worth using the two methods and to compare the values obtained for both D_2 and C.

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