Doklady Physics, Vol. 47, No. 8, 2002, pp. 620–622. Translated from Doklady Akademii Nauk, Vol. 385, No. 4, 2002, pp. 494–496.

MECHANICS

Peculiarities of the Bending-Stiffness Calculation for Nanocrystals

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Received March 12, 2002

In view of the evolution of nanotechnology, it is of current interest to develop analytical models for describing the mechanical deformation of nanodimensional objects. The majority of available theoretical models are based on elasticity-theory equations. In this case, values of the modulus of elasticity obtained in macroscopic experiments are commonly used. At the same time, many investigators pointed to a discrepancy between values of the modulus of elasticity obtained in microscopic and macroscopic experiments (see, e.g., [1–3]). In [4], the Young's modulus and Poisson's ratio were theoretically investigated as functions of the number of atomic layers by the example of a two-dimensional single-crystal strip. It was shown that, with a decreasing number of atomic layers, the Poisson's ratio decreases and the Young's modulus increases and, for two-layer crystalline films, can differ from their macroscopic values by a factor of 1/2 and 2, respectively. The results [4] indicate that scale effects must be taken into account when notions of continuum mechanics are applied to nano-objects. In this study, we theoretically investigated the effect of the scale factor on the bending stiffness of a single-crystal strip. This problem is of high priority because, in particular, it is necessary to investigate the stress–strain state of nanotubes, which are extensively used in current engineering applications [5–8].

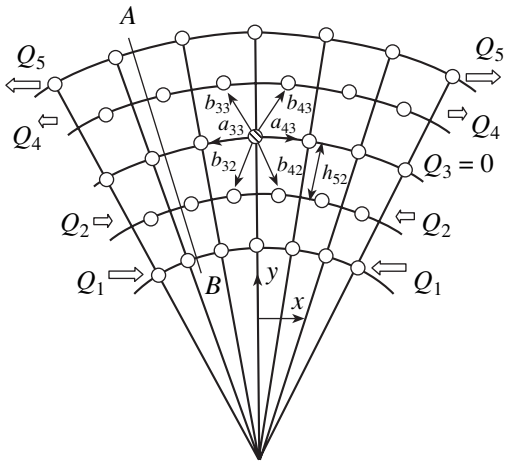
We consider a two-dimensional single crystal with $N \geq 2$ layers along the y axis and $J \gg N$ layers along the x axis. Each atom is assumed to interact only with the nearest neighbors (see figure). Forces Q_n are applied to the atoms on the lateral faces of the crystal. The subscript n means the layer number ($n = 1, 2, \ldots, N$). From one layer to another, forces vary linearly, so that the summary load acting on the lateral crystal face provides only the moment of force

$$\sum_{n=1}^{N} Q_n = 0, \quad \sum_{n=1}^{N} R_n Q_n = M. \tag{1}$$

The strained state of the single crystal is completely specified by spacings a_{jn} between the neighboring atoms in each layer and by spacings b_{jn} between the nearest atoms in the neighboring layers. The subscripts j and n correspond to the numbers of layers along the x and y axes, respectively (see figure). It is evident that spacings h_{jn} between layers can be determined from the geometric relationship $h_{jn}^2 = b_{jn}^2 - \frac{a_{jn}^2}{4}$. In the unstrained state, the crystal lattice consists of equilateral triangles with sides $a = b = a_0$. This lattice is characterized by the relations

$$h_0 = \frac{\sqrt{3}}{2} a_0, \quad R_n = (n-1)h_0.$$

It is easy to show that the formula for Q_n satisfying



Bending of a nanocrystal strip.

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conditions (1) has the form

$$Q_n = \frac{4\sqrt{3}M(2n-N-1)}{a_0(N-1)N(N+1)}. \quad (2)$$

Let $F(r)$ be the force of interaction between two atoms separated by distance r. Assuming the smallness of strains (displacements are magnified in the figure for clearness) induced by the forces of interaction between atoms in the crystal, we use the linear approximation

$$F(a_{jn}) = C\Delta a_{jn}, \quad F(b_{jn}) = C\Delta b_{jn}, \quad C \stackrel{\text{def}}{=} F'(a_0) > 0, \quad (3)$$

where C is the interatomic-bond rigidity, $\Delta a_{jn} \stackrel{\text{def}}{=} a_{jn} - a_0$, and $\Delta b_{jn} \stackrel{\text{def}}{=} b_{jn} - a_0$. Such a simplified approach is justified by the fact that the modulus of elasticity in continuum mechanics is generally determined in linear theory. It should be noted that the approach proposed here can be realized even without the assumption that elastic bonds are linear; the difficulties arising in this case are of a purely technical nature. Writing the equations of equilibrium for atoms of the crystal lattice, we obtain the set of recurrence equations for the quantities Δa_{jn}, Δb_{jn}, and Q_n:

$$\Delta a_{j,n} + \frac{1}{2}(\Delta b_{j,n} + \Delta b_{j,n-1}) = \Delta a_{j-1,n} + \frac{1}{2}(\Delta b_{j-1,n} + \Delta b_{j-1,n-1}),$$

$$\Delta b_{j,n} + \Delta b_{j-1,n} = \Delta b_{j,n-1} + \Delta b_{j-1,n-1}, \quad (4)$$

$$\Delta a_{l,n} + \frac{1}{2}(\Delta b_{l,n} - \Delta b_{l-1,n} + \Delta b_{l,n-1} - \Delta b_{l-1,n-1}) = \frac{Q_n}{C},$$

$$\Delta a_{J-l,n} + \frac{1}{2}(\Delta b_{J-l,n} - \Delta b_{J-l+1,n} + \Delta b_{J-l,n-1} - \Delta b_{J-l+1,n-1}) = \frac{Q_n}{C}, \quad l = 1, 2.$$

The solution to these equations has the form

$$\Delta b_{jn} = 0, \quad \Delta a_{jn} = \frac{Q_n}{C}. \quad (5)$$

We conceptually cut the crystal by a vertical straight line AB (see figure). According to Eqs. (2) and (5), the total normal force acting from one part of the crystal to the other is equal to zero. The total bending moment M is calculated by Eq. (1). As can be seen from Eqs. (2) and (5), a change in interatomic spacings Δa_{jn} linearly depends on the layer number n along the y axis and is independent of the layer number j along the x axis. This means that the atomic layers along the y axis remain rectilinear when the crystal is deformed, and the angles between any neighboring atomic layers in the strained state are identical. In this case, the angle α between the neighboring atomic layers and the corresponding curvature β are determined as follows:

$$\alpha \stackrel{\text{def}}{=} \frac{\Delta a_{jN}/2 - \Delta a_{j1}/2}{h_0(N-1)}, \quad \beta \stackrel{\text{def}}{=} \frac{\alpha}{a_0/2}. \quad (6)$$

According to Eqs. (2), (5), and (6), the bending stiffness of the single-crystal strip has the form

$$D \stackrel{\text{def}}{=} \frac{M}{\beta} = \frac{Ca_0^3}{16}(N-1)N(N+1). \quad (7)$$

Attempts to express bending stiffness in terms of macroscopic parameters encounter difficulties associated with the possibility of different definitions of the thickness H of the nanocrystal. On the one hand, the single-crystal thickness can be defined as the spacing $H = (N-1)h_0$ between atomic layers at opposite ends; on the other hand, the nanocrystal thickness can be defined as the product of the number of layers and the thickness of one atomic layer: $H = Nh_0$. Because it is difficult to give preference to one of the formulated definitions, we define nanocrystal thickness as [4]

$$H \stackrel{\text{def}}{=} N_* h_0, \quad N - 1 \le N_* \le N, \quad (8)$$

where N_* is a dimensionless parameter reflecting the ambiguity in the determination of H. As is shown in [4], the Young's modulus E_1 corresponding to extension along the x axis of a single-crystal strip, which is infinite in this direction, is calculated by the formula

$$E_1 = \frac{N}{N_*}E_\infty, \quad E_\infty = \frac{2C}{\sqrt{3}}. \quad (9)$$

Here, E_∞ is the Young's modulus of the infinite crystal [9, 10]. It should be noted that we consider a strip finite along the x axis. However, the number of atomic layers along this direction is assumed to be so large that Eq. (9) can be used. Using Eqs. (8) and (9), we express bending stiffness (7) of the single-crystal strip in terms of its macroscopic parameters:

$$D = \frac{E_1 H^3(N^2-1)}{12N_*^2}. \quad (10)$$

Experimental data indicate that the bending stiffness of a single-layer strip is 25 times lower than the value obtained by the formula of elasticity theory [11]. Indeed, a single-layer chain of atoms must have no bending stiffness from the classical viewpoint. Therefore, it should be considered that the most acceptable values of N_* in bending problems are those for which the bending stiffness D vanishes at $N = 1$ (a low experimentally observed bending stiffness is associated with the effects ignored in the model under consideration). We consider two N_*-values satisfying the above condition.

First, we assume that $N_* = N$. In this case, $E_1 = E_\infty$ and bending stiffness is defined by the formula

$$D = D_\infty\left(1 - \frac{1}{N^2}\right), \quad D_\infty = \frac{E_\infty H^3}{12}, \quad H = Nh_0. \quad (11)$$

Here, D_∞ is the bending stiffness of the strip known from macroscopic elasticity theory. According to Eq. (11), the bending stiffness of the nanocrystal varies within the interval $0 \le D \le D_\infty$. For small N, this stiffness substantially depends on the number of atomic layers. It increases with N and tends to its elasticity-theory value for $N \longrightarrow \infty$.

On the other hand, we assume that

$$N_* = N\left(1 - \frac{1}{N^2}\right)^{1/3}.$$

The parameter N_* introduced in such a way satisfies inequality (8): $N - 1 \le N_* \le N$. In this case, the bending stiffness and the thickness of the nanocrystal are expressed as

$$D = \frac{E_\infty H^3}{12} \equiv D_\infty, \quad H = Nh_0\left(1 - \frac{1}{N^2}\right)^{1/3}. \quad (12)$$

It is easy to see that the expression for bending stiffness exactly coincides with the elasticity-theory expression. The strip-thickness expression coincides, for large N, with Nh_0 corresponding to the previous case. For small N, Eq. (12) gives thickness values lower than Nh_0; for $N = 1$, it vanishes as it must according to the concept that a single-atom layer has zero bending stiffness.

An alternative way of determining bending stiffness is to solve the problem of the deformation of a single-crystal strip upon its bending into a ring. This problem can be considered as linear in strains; however, it is geometrically nonlinear in displacements. An advantage of this formulation is the fact that it requires no assumptions about the nature of the external load. The expressions for bending stiffness D obtained as a result of solving the similar problem coincide exactly with Eqs. (10)–(12).

The problem of determining the bending stiffness of nanotubes was considered in the quasi-continuum formulation in [5], where, for several particular N-values, a strip bending stiffness which coincided with the results calculated by Eq. (11) was determined. Strip thickness was defined in [5] as $H = h_0N$, which is responsible for the discrepancy between bending stiffness and its elasticity-theory value. However, as was shown above, the application of the alternative definition of plate thickness makes it possible to use the macroscopic formula for bending stiffness without any modifications.

ACKNOWLEDGMENTS

This study was supported by the Russian Foundation for Basic Research (project no. 02-01-00514).

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Translated by V. Bukhanov