

Anomalies in Mechanical Characteristics of Nanometer-Size Objects

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Received July 18, 2001

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. In particular, one of the methods of determining elastic characteristics of nanosize objects is investigating the microrelief arising in the course of tension of a specimen having an ultrathin coating [1–3]. The solution to an equivalent continual problem allows the Poisson's ratio and Young modulus for the coating to be determined from such experiments [2, 4, 5]. However, the values of elastic characteristics measured by this method exhibit a substantial inconsistency by their macroscopic values for the same material.

In the present study, we used a two-dimensional strip made of a single-crystal material with a hexagonal closely packed (HCP) lattice as a model for studying the effect of scaling on mechanical properties of a material. The interaction between atoms is assumed to be dual. The basic problem of our study is determining the dependence of the Poisson's ratio and Young modulus of a finite (in one direction) single crystal on the number of atomic layers.

We consider a two-dimensional single crystal shown in the figure. The crystal possesses an infinite length along the x direction and $N \geq 2$ atomic layers in the y direction. Each atom interacts only with its nearest neighbors, as is shown in the figure. 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 . We denote by the symbol b the distance between nearest atoms in neighboring layers (see figure). In this case, evidently, the relationship $b^2 = \frac{a^2}{4} + h^2$ is valid. In the undistorted state, the lattice consists of equilateral triangles with an edge $a = b = a_0$, and the end load is absent ($Q = 0$). Let $F(r)$ be the force of interaction between two atoms separated by distance r (the attraction is considered as positive). Then, projecting onto the y direction the equation of equilibrium for an atom situated at the crystal surface, we find

$$Q = 2\frac{h}{b}F(b) \Rightarrow \sigma_2 \stackrel{\text{def}}{=} \frac{Q}{a} = 2\frac{h}{ab}F(b). \quad (1)$$

Here, σ_2 is the normal stress in the y direction. We now mentally cut the crystal by a vertical straight line AB (see figure). The total normal force acting from one part of the crystal onto the other part can be written out as

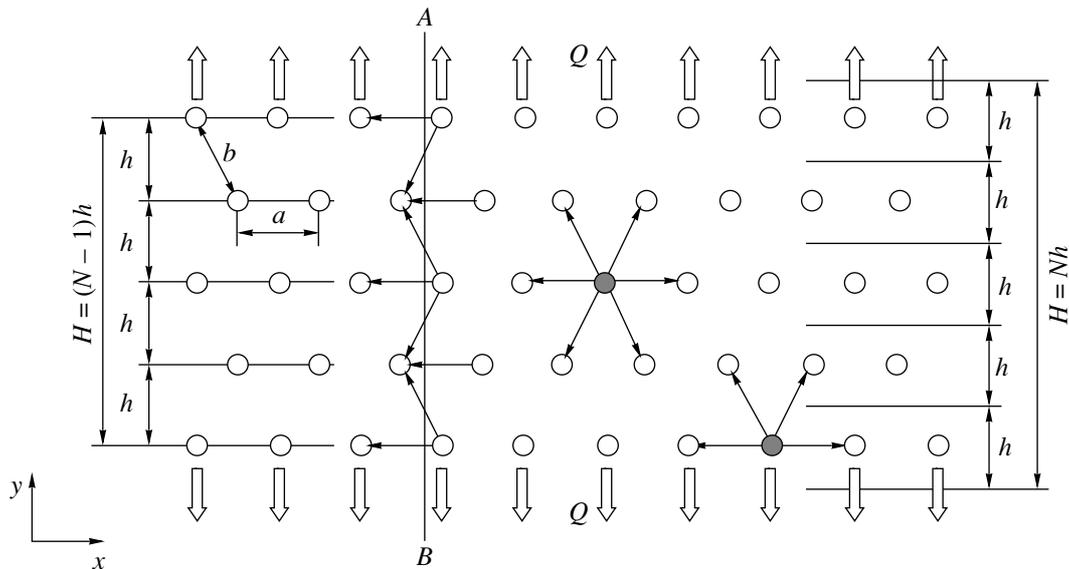
$$H\sigma_1 = NF(a) + (N-1)\frac{a}{2b}F(b). \quad (1a)$$

Here, σ_1 is the normal stress in the x direction and H is the crystal thickness (its extension along the y direction). The quantity H , 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 figure), 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

$$H \stackrel{\text{def}}{=} N_*h, \quad N-1 \leq N_* \leq N, \quad (2)$$

where N_* is the quantity reflecting an arbitrariness in the determination of H . By virtue of the smallness of

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Two-dimensional single-crystal strip.

strains, forces acting within the crystal can be approximately written out in the form

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

where C has a meaning of the rigidity of an interatomic bond, while the symbol Δ implies the deviation of a certain quantity from its value corresponding to the undistorted crystal. We denote the crystal strain in the x and y directions as ε_1 and ε_2 , where

$$\varepsilon_1 \stackrel{\text{def}}{=} \frac{\Delta a}{a_0}, \quad \varepsilon_2 \stackrel{\text{def}}{=} \frac{\Delta h}{h_0}, \quad h_0 \equiv \frac{\sqrt{3}a_0}{2}. \quad (4)$$

The substitution of relationships (2), (3), and (4) into expressions (1) and (1a) yields the elasticity relations

$$\begin{aligned} \sigma_1 &= \frac{\sqrt{3}}{12} \frac{C}{N_*} ((9N-1)\varepsilon_1 + 3(N-1)\varepsilon_2), \\ \sigma_2 &= \frac{\sqrt{3}}{4} C(\varepsilon_1 + 3\varepsilon_2). \end{aligned} \quad (5)$$

As is seen from relations (5), 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. Furthermore, we denote

$$\begin{aligned} \nu_1 &\stackrel{\text{def}}{=} -\left. \frac{\varepsilon_2}{\varepsilon_1} \right|_{\sigma_2=0}, \quad E_1 \stackrel{\text{def}}{=} \left. \frac{\sigma_1}{\varepsilon_1} \right|_{\sigma_2=0}; \\ \nu_2 &\stackrel{\text{def}}{=} -\left. \frac{\varepsilon_1}{\varepsilon_2} \right|_{\sigma_1=0}, \quad E_2 \stackrel{\text{def}}{=} \left. \frac{\sigma_2}{\varepsilon_2} \right|_{\sigma_1=0}. \end{aligned}$$

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 (5), we obtain

$$\begin{aligned} \nu_1 &= \nu_\infty, \quad E_1 = \frac{N}{N_*} E_\infty; \\ \nu_2 &= \frac{N-1}{N-1/9} \nu_\infty, \quad E_2 = \frac{N}{N-1/9} E_\infty, \end{aligned}$$

where, $\nu_\infty = \frac{1}{3}$ and $E_\infty = \frac{2C}{\sqrt{3}}$ are values of the Poisson's ratio and Young modulus, which correspond to the infinite crystal [6, 7]. We now analyze the formulas obtained. Under tension along atomic layers, the Young modulus E_1 substantially depends on the quantity N_* , i.e., on a method for determining the thickness of the nanocrystal strip. If we assume that $N_* = N$ (N is the maximal value of N_*) then, under tension along atomic layers, the Poisson's ratio and Young modulus are independent of a number of layers. Evidently, this is associated with the fact that in the longitudinal direction, the crystal under consideration is infinite. By contrast, the Young modulus E_1^{max} corresponding to the minimal value $N_* = N - 1$, is not constant. It increases with a decrease in the number of atomic layers and for $N = 2$ attains a value twice as large as E_∞ (see table). Thus, the ambiguity in determining the Young modulus turns out to be rather substantial for small values of N . In the case of tension in the direction perpendicular to atomic layers, both the Poisson's ratio and the Young modulus depend on N , the former decreasing and the latter

increasing with the reduction in the number of layers. The values of the Poisson's ratio and Young modulus for different N are presented in the table. It is worth noting that for $N = 2$ the Poisson's ratio is smaller than ν_∞ almost by a factor of 2. As $N \rightarrow \infty$, elastic moduli tend to values corresponding to the infinite crystal, which are independent of the deformation direction.

Based on the studies performed, we can list the basic properties intrinsic to nanocrystals.

1. For the Young modulus 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.

The effects listed are obtained on the basis of a rather simplified model. However, as far as they manifest themselves for the simplest nanocrystal, they must all the more play an important role in the case of more complicated nanocrystalline objects. The indicated ambiguity in the determination of the Young modulus, evidently, manifests itself for all mechanical characteristics whose definition substantially involves the concept of the nanoobject's size. In particular, the specific deformation energy per unit volume is determined ambiguously.

In the present study, we took into account the interaction of only neighboring atoms in the crystal lattice. It can be shown that allowance for further neighbors leads to the enhanced effect of the scale factor, especially in the three-dimensional case.

Thus, the concepts of classical continuum mechanics, including those of the elasticity theory, must be used with great care in the case of their application to nanoobjects. It is necessary to take into account the variation of mechanical characteristics when scales of objects under consideration approach nanometers. Special attention should be paid to quantities (such as the Young modulus) that are in principle ambiguous at the nanometer level. Using them, we must clearly define

Poisson's ratio and Young modulus of a nanocrystal as functions of the number of atomic layer

N	E_1^{\max}/E_∞	ν_2	ν_2/ν_∞	E_2/E_∞
2	2.00	0.18	0.53	1.06
3	1.50	0.23	0.69	1.04
4	1.33	0.26	0.77	1.03
5	1.25	0.27	0.82	1.02
10	1.11	0.30	0.91	1.01
20	1.05	0.32	0.96	1.01
50	1.02	0.33	0.98	1.00
100	1.01	0.33	0.99	1.00

what we imply while applying these quantities to nanoobjects.

ACKNOWLEDGMENTS

This work was supported by the Russian Foundation for Basic Research, project nos. 9907-90443 and 0001-00489.

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Translated by G. Merzon