Solid mechanics methods in nano-technologies

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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 nanometersize (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 to investigate theoretically 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 twodimensional single crystal shown in the Figure 1. The crystal possesses an infinite length along the x direction and $N \geq 2$ atomic layers in the direction. Each atom interacts only with its nearest neighbors, as is shown in the Figure 1. Constant tensile

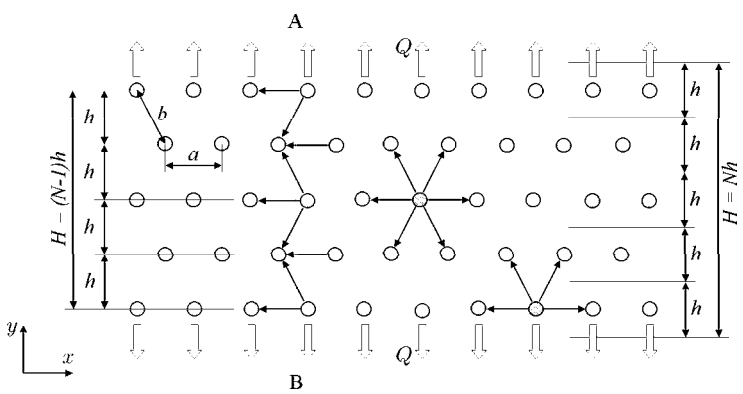

Figure 1:

forces Q are applied to atoms located at crystal ends. The deformed singlecrystal 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 Figure 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 $H = N_*h$, $N - 1 \leq N_* \leq N$, 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. Furthermore, we denote

$$\nu_1 = -\left.\frac{\epsilon_2}{\epsilon_1}\right|_{\sigma_2=0} \qquad E_1 = \left.\frac{\sigma_1}{\epsilon_1}\right|_{\sigma_2=0} \qquad \nu_2 = -\left.\frac{\epsilon_1}{\epsilon_2}\right|_{\sigma_1=0} \qquad E_2 = \left.\frac{\sigma_2}{\epsilon_2}\right|_{\sigma_1=0}. \tag{1}$$

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

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

where, ν_∞ and E_∞ are values of the Poisson's ratio and Young modulus, which correspond to the infinite crystal.

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 Figure 2. The crystal possesses $N \geq 1$ atomic layers in the y direction and $J \gg N$ layers in the x direction. Forces Q_n

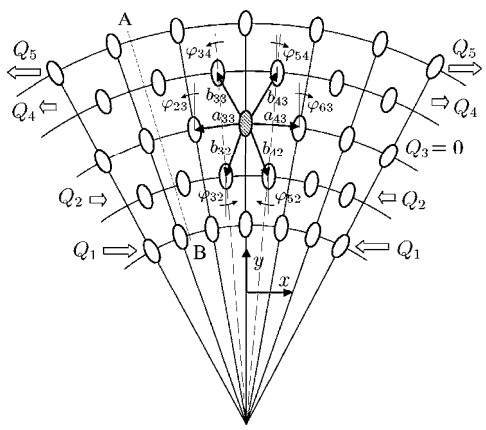

Figure 2:

are applied to atoms located at crystal end-walls, where n is the number of the horizontal layer, containing 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

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

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

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

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 $N = 1$.

The model of the delamination processes of a preliminary stressed bi-layered plate from rigid foundation is proposed. On the basis of the considered solution of specified dependence of its diameter on the parameters of plate layers is found.