STRENGTH AND STABILITY OF NANOOBJECTS

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ABSTRACT

Advances in high technologies using nanometer-size structures, such as thin films and carbon nanotubes, requires calculation of mechanical properties for the objects of the nanosize scale level. Majority of the theoretical mechanical models for nanoobjects is based on the macroscopic equations of theory of elasticity. This gives the questions about applicability of the quantities obtained from the macroscopic experiments to the nanoscale objects or about necessity of corrections taking into account the scale effects. The presented paper is devoted to 1) theoretical investigation of the influence of the scale effects on the Poisson's ratio, Young modulus and the bending stiffness of a nanocrystal, which is extended in one direction and has a limited number of atomic layers in another direction, 2) theoretical investigation of the delamination processes of a preliminary stressed bi-layered plate from a rigid foundation, 3) creation of stable models for crystal lattices.

1 INTRODUCTION

In recent years, rapid development of nanotechnologies led to the necessity of constructing adequate physical models for describing physico-mechanical properties of objects with a nanometer-size (nanosize) scale. The majority of the existing models of such a kind assume that the 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 1) to investigate theoretically the scale effect for the Poisson's ratio, Young modulus and the bending stiffness of thin nanocrystalline structures, 2) to investigate the delamination processes of a preliminary stressed bi-layered plate from rigid foundation, 3) to propose the method of creation of stable models of crystal lattices. 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 (Ru [1], Prinz [2]). 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.

2 POISSON'S RATIO AND YOUNG MODULUS DETERMINATION

We consider a two-dimensional single crystal shown in Figure 1. The crystal possesses an infinite length along x direction and $N \geq 2$ atomic layers in y direction. Each atom interacts only with its nearest neighbors, as it is shown in Figure 1. Constant tensile forces Q are applied to atoms located at the 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 y direction), in principle, cannot be determined unambiguously. For example, if we assume that the crystal thickness is equal to the distance between the atomic layers lying on the opposite crystal ends (see Figure 1) then $H = (N-1)h$. 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 let us denote $H = N^* h$, $N - 1 \le N^* \le N$, where N^* is the quantity reflecting an arbitrariness in the determination of H.

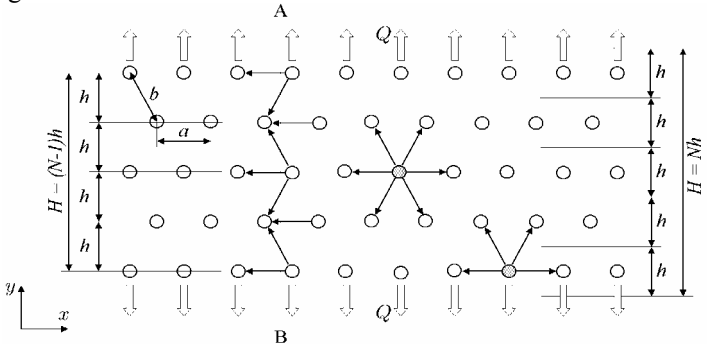

Figure 1: Two-dimensional single-crystal strip.

It can be easily shown that 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

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

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

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

where, ν_∞ and E_∞ are values of the Poisson's ratio and Young modulus, which correspond to the infinite crystal (Krivtsov [3]).

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.

3 THE BENDING STIFFNESS DETERMINATION

Let us consider a two-dimensional single crystal shown in Figure 2. The crystal possesses $N \ge 2$ atomic layers in y direction and $J >> N$ layers in x direction. Forces Q_n 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).

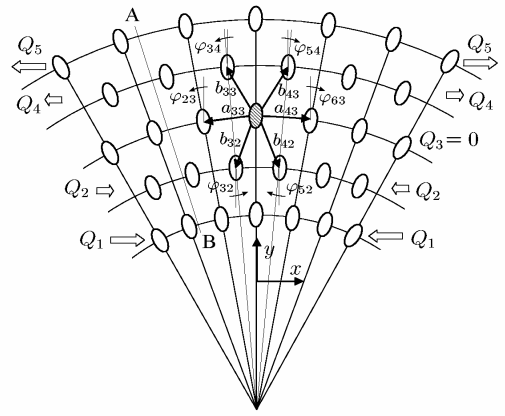

Figure 2: Bending of the nanocrystalline strip.

If the moment interaction between the particles is not taken into account then the bending stiffness of the monocrystal takes the form

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

Here D_∞ is the value for the bending stiffness from the macroscopic theory of elasticity. According to formula (3), for the small values of N the bending stiffness depends essentially on the number of the layers. For the greater 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 is not 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 vanish for $N = 1$.

4 DELAMINATION PROCESSES OF A BI-LAYERED PLATE

The model of the delamination processes of a preliminary stressed bi-layered plate from a rigid foundation is proposed. A thin bi-layered plate is considered. Let h_1, E_1, ν_1 and h_2, E_2, ν_2 be the thickness, Young modulus and the Poisson's ratio of the plate layers and L be the plate length. The first layer is attached to the rigid foundation. The second layer has initial deformation ε_0 and it is attached to the first layer. Let us suppose that part of the plate comes off the rigid foundation and rolls up. In this paper the process of the bi-layered plate rolling up is simulated on the basis of

the classical Lagrange's equations. Process of bi-layered plate delamination is considered as a damage process, which is caused by weakening of the connection between the bi-layered plate and the rigid foundation. On the basis of the considered solution, specified dependence of the tube radius on the parameters of the plate layers is found

$$R_* = \frac{(1+\xi)h_1}{2p\varepsilon\xi_0\eta}, \quad \xi = \frac{h_1}{h_2}, \quad \eta = \frac{\mathrm{E}_2(1-\nu_1^2)}{\mathrm{E}_1(1-\nu_2^2)}, \quad p = \frac{3(1+\xi)^2}{1+(4+6\xi+4\xi^2)\eta+\xi^4\eta^2} \qquad (5)$$

Dynamic equations, which describe delamination processes of a preliminary stressed bi-layered plate from the rigid foundation, is obtained using Lagrange's equations. Kinetic energy of the plate is

$$T = (\rho_1 h_1 + \rho_2 h_2)\left(l - R\sin\frac{l}{R}\right)\left[\left(\frac{dl}{dt}\right)^2 + \left(\frac{dR}{dt}\right)^2\right] \qquad (6)$$

Here ρ_1 and ρ_2 are density of the plate layers, l is the length of the rolled part of the plate. Potential energy of the plate, which part is rolled in a tube, takes the form

$$\Pi = \left(1 - \frac{\xi\eta}{1+\xi\eta}\right)\Pi_0 - \frac{\xi\eta}{1+\xi\eta}\frac{R_*}{R}\left(2 - \frac{R_*}{R}\right)p, \qquad \Pi_0 = \frac{E_2 h_2 \varepsilon_0^2}{2(1-\nu_2^2)} \qquad (7)$$

Let us write Lagrange's equations, considering l and R as generalized coordinates. Using new variables

$$\varphi = \frac{l}{R_*}, \qquad r = \frac{R}{R_*}, \qquad \tau = t\omega, \qquad \omega^2 = \frac{\Pi_0\xi\eta}{(\rho_1 h_1 + \rho_2 h_2)R_*^2(1+\xi\eta)}, \qquad (8)$$

we obtain the differential equation, describing the bi-layered plate rolling process

$$2\varphi''\left(\varphi - r\sin\frac{\varphi}{r}\right) + \left([\varphi']^2 - [r']^2\right)\left(1 - \cos\frac{\varphi}{r}\right) - \frac{2r'\varphi'}{r}\left(r\sin\frac{\varphi}{r} - \varphi\cos\frac{\varphi}{r}\right) = q(1+p) - \frac{p(1-r)^2}{r^2}$$

$$2r''\left(\varphi - r\sin\frac{\varphi}{r}\right) - \left([\varphi']^2 - [r']^2\right)\left(\frac{\varphi}{r}\cos\frac{\varphi}{r} - \sin\frac{\varphi}{r}\right) - 2\varphi' r'\left(1 - \cos\frac{\varphi}{r}\right) = \frac{2p\varphi(1-r)}{r^3}$$

Here prime stands for the derivative with respect to τ. Numerical analysis of the system of differential equations (9) is carried out.

5 DESCRIPTION OF CRYSTAL LATTICE (MOMENT THEORY)

Pair potentials, describing interaction of particles, are widely used for simulation of molecular systems. Physical sense of these potentials is clear and they allow qualitatively description of the material properties. However, it is known, that these potentials can not guarantee stability for many crystal lattices. Traditional solution of the problem is to apply many-body potentials (Tersoff [4], Brenner [5]). In the presented paper alternative approach is proposed. The main idea of the approach is to consider the atoms as particles of general kind (not material points) and take into account the moment interaction between the particles.

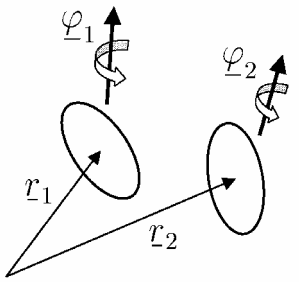

Figure 3: Moment interaction of particles.

Let us consider two such particles, as depicted in Figure 3. Let us suppose that interaction between the particles depends on their position and orientation. The Interaction is characterized by the force vector $\underline{F}$ and the moment vector $\underline{M}$

$$\underline{F} = \frac{\partial U}{\partial \underline{\varepsilon}}, \qquad \underline{M} = \frac{\partial U}{\partial \underline{\kappa}}, \tag{6}$$

where elastic energy U and strain vectors $\underline{\varepsilon}$ and $\underline{\kappa}$ take the following form

$$U = \frac{1}{2}\underline{\varepsilon}\cdot\underline{\underline{A}}\cdot\underline{\varepsilon} + \underline{\varepsilon}\cdot\underline{\underline{B}}\cdot\underline{\kappa} + \frac{1}{2}\underline{\kappa}\cdot\underline{\underline{C}}\cdot\underline{\kappa}, \tag{7}$$

$$\varepsilon = \underline{r} - \underline{r}_0 + \frac{1}{2}\underline{r}_0 \times (\underline{\varphi}_1 + \underline{\varphi}_2), \qquad \underline{\kappa} = \underline{\varphi}_2 - \underline{\varphi}_1, \qquad \underline{r} = \underline{r}_2 - \underline{r}_1.$$

Coefficients $\underline{\underline{A}}$, $\underline{\underline{B}}$, $\underline{\underline{C}}$ are stiffness tensors. Let us consider ideal simple crystal lattice consisting of the particles of general kind. Let $\underline{a}_\alpha$ be vector characterizing position of the particle number α with respect to the considered particle in the reference position. Interaction of the considered particle and the particle number α is characterized by stiffness tensors

$$\underline{\underline{A}}_\alpha = \sum_{n=1}^{3} A_{\alpha n}\,\underline{e}_n\,\underline{e}_n, \qquad \underline{\underline{B}}_\alpha = 0, \qquad \underline{\underline{C}}_\alpha = \sum_{n=1}^{3} C_{\alpha n}\,\underline{e}_n\,\underline{e}_n, , \tag{8}$$

where $\underline{e}_n$ are eigen-vectors of $\underline{\underline{A}}_\alpha$ и $\underline{\underline{C}}_\alpha$. Equations of dynamics for crystal packing of particles with rotational degrees of freedom are obtained. It is shown that in a long-wave approximation these equations are identical to macroscopic equations of the moment theory of elasticity. The expressions for stiffness tensors of the crystal lattice are

$$\begin{gathered}{}^4\underline{\underline{A}}_* = \frac{1}{2V_*}\sum_\alpha\sum_{n=1}^{3} A_{\alpha n}\underline{e}_n\underline{a}_\alpha\underline{e}_n\underline{a}_\alpha, \qquad {}^4\underline{\underline{C}}_* = \frac{1}{2V_*}\sum_\alpha\sum_{n=1}^{3} C_{\alpha n}\underline{e}_n\underline{a}_\alpha\underline{e}_n\underline{a}_\alpha, \\ {}^4\underline{\underline{B}}_* = \frac{1}{4V_*}\sum_\alpha\sum_{n=1}^{3} A_{\alpha n}\underline{e}_n\underline{a}_\alpha\underline{e}_n\times\underline{a}_\alpha\underline{a}_\alpha.\end{gathered}, \tag{9}$$

where V_* is volume of the elementary cell. It is easy to see that the stiffness tensors of the crystal lattice depend on the crystal lattice configuration and parameters, characterizing stiffness of the atom connection.

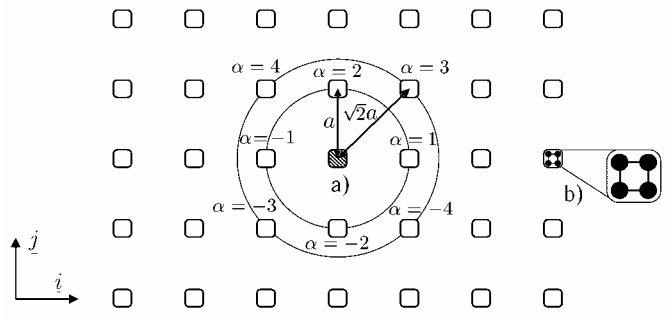

Figure 4: Square crystal lattice.

As an example the square crystal lattice is considered (see Figure 4). It is shown, that modeling the atoms by the particles of general kind allows stabilizing this lattice. The simplest model of the particle taking into account symmetry of the square lattice is proposed. This model is a rigid body, which consists from four material points, situated in the corners of the square (see Figure 4). Areas of the lattice stability are obtained for the considered model.

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