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Selected Problems of Nanomechanics

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Abstract: In a study of nanoscale objects it is important to consider the growing influence of the surface. A number of classical problems of elasticity for nanoscale structures is considered taking into account surface stresses. The results of analysis are compared to classical results. The effects of taking into account surface stresses on the effective stiffness of nanoporous rod and on the stability of a plate with a circular cut in tension are investigated

Keywords: nanomaterials, nanoscale objects, surface stress.

1 Introduction

A starting year for nanomechanics in St. Petersburg can be considered 2000, the year when Zhores Alferov won his Nobel prize. Lectures that were delivered by tradition in St. Petersburg afterwards and were devoted to this event, aroused a serious scientific interest towards a range of problems bounded with nanotechnology among different scientists, including mechanicians. The study of mechanical properties of solid nanoobjects has shown that the same range of problems as that of the objects on traditional scale can be attributed to them: strength, fracture, defectiveness, delamination, stability, hence in order to predict their behavior theoretical models should be used. It is natural for mechanicians to choose classical models for a study of materials and constructions, including respective modifications into them, and the first problem here is defining basic parameters such as Young's modulus and Poisson's ratio. Some of the results regarding ambiguity in defining Young's modulus for a small amount of atomic layers are given in [1, 2].

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2 On surface effects

A variety of nanomaterials possess physical properties that are considerably different from those of usual materials. One of the explanations would be presence of surface effects, the role of which in the case of nanoscale structures can be significant in comparison to the classical mechanics. As a model that considers surface properties theory of elasticity with surface stresses[3-7] can be taken. Surface stresses τ are a generalization of surface tension, notable in the theory of capillarity, in the case of solid materials. Within its framework together with stress tensor σ, defined inside the solid's volume V and on its surface Ω, surface stresses τ act on the solid's surface or on a part of it. Tensor τ generalizes the scalar surface stress known in fluid mechanics for the case of solids. Introduction of surface stress would allow to define size effect that is typical for nanomaterials.

Mathematical investigations of surface stresses in solids and fluids are to be found in the works by Laplace, Young, Gibbs et al., see, for example, surveys in [8,9]. Equilibrium equations and boundary conditions for a linearly elastic body with surface stresses are as follows in [3-8]

$$\begin{aligned} &\nabla\cdot\sigma+\rho\mathbf{f}=0 \text{ in } V \\ &\mathbf{u}|_{\Omega_d}=\mathbf{u}_0,\ \ \mathbf{n}\cdot\sigma|_{\ \Omega_f}=\varphi,\ \ (\mathbf{n}\cdot\sigma-\nabla_S\cdot\tau)|_{\ \Omega_S}=\varphi \end{aligned} \tag{1}$$

In (1) σ are stresses, ∇ is a differential operator in three dimensions,ρ is density, $\mathbf{f}$ are mass forces, $\mathbf{n}$ is a normal to a surface of a body, $\Omega\equiv\partial V=\Omega_d\cup\Omega_f\cup\Omega_S$, at Ω_d the displacements $\mathbf{u_0}$ are given, Ω_f is exposed to forces φ, meanwhile Ω_S is also exposed to surface stresses τ ∇_S is a surface operator of a gradient, connected with ∇ by $\nabla_S=\nabla-\mathbf{n}\frac{\partial}{\partial z}$, z is a coordinate counted by a normal to a surface Ω. Stress tensors and surface stress tensors in (1) are given by

$$\begin{aligned} &\sigma=\tfrac{\partial W}{\partial\varepsilon}=\lambda\mathbf{I}tr\varepsilon+2\mu\varepsilon, \\ &\tau=\tfrac{\partial U}{\partial\varepsilon}=\tau_0\mathbf{A}+\lambda^S\mathbf{I}tr\varepsilon+2\mu^S\varepsilon, \end{aligned} \tag{2}$$

$$\begin{aligned} &W=W(\varepsilon)=\tfrac{1}{2}\lambda\mathbf{I}(tr\varepsilon)^2+\mu\varepsilon\cdot\cdot\varepsilon, \\ &\varepsilon=\varepsilon(\mathbf{u})\equiv\tfrac{1}{2}(\nabla\mathbf{u}+\nabla\mathbf{u^T}), \end{aligned} \tag{3}$$

$$\begin{aligned} &U=U(\varepsilon)=\tau_0 tr\varepsilon_\mathbf{S}+\tfrac{1}{2}\lambda^S\mathbf{I}(tr\varepsilon_S)^2+\mu\varepsilon_S\cdot\cdot\varepsilon_S, \\ &\varepsilon_\mathbf{S}=\varepsilon_\mathbf{S}(\mathbf{u})\equiv\tfrac{1}{2}((\nabla_\mathbf{S}\mathbf{u_S})\cdot\mathbf{A}+\mathbf{A}\cdot(\nabla_\mathbf{S}\mathbf{u_S})^\mathbf{T}) \end{aligned} \tag{4}$$

Here ε is a bulk strain tensor, ε_S is a surface strain tensor, $\mathbf{u}_S=\mathbf{u}|_{\Omega_S}$ is a displacements vector at Ω_S, $\mathbf{A}=\mathbf{I}-\mathbf{n}\otimes\mathbf{n}$, $\mathbf{I}$ is a unity tensor in three dimensions, λ and μ are Lamé parameters, λ^S and μ^S are surface Lamé parameters, τ_0 is a residual surface stress.

3 Effective Stiffness Parameters of a Nanoporous Rod

Let's consider a problem of tension of a linear elastic rectilinear rod with a circular cross-section having a radius R. Consider that paralleled to the rod axis there exist rectilinear n cylindrically shaped pores with an equal radius r with a total area of their cross sections equal to

$$S = \pi n r^2 \tag{5}$$

Let an equally distributed load act on ends of the rod being statistically equivalent to forces P. By designating Young modulus as E, an effective longitudinal modulus of a rod with pores E_0^* can be given as follows:

$$E_0^* = E(1-\varphi) \tag{6}$$

Here $\varphi = S/F$ is porosity, $F = \pi R^2$ is a total area of the rod's cross-section including the area of the pores. Obviously the effective longitudinal E_0^* does not depend on the quantity of pores in it but only on the total area of their cross-sections.

The effective elastic modulus with taken into account surface stresses E_S^* can be expressed as

$$E_S^* = E(1-\varphi) + E_S \frac{2\pi r n}{F} = E_0^* + E_S \frac{2\pi r n}{F} \tag{7}$$

or considering (5)

$$E_S^* = E(1-\varphi) + E_S \frac{2\sqrt{S}}{2\sqrt{\pi F}} \sqrt{n} \tag{8}$$

Here $E_S = \sigma_{zz}/\varepsilon_{zz} > 0$ is a surface analogue to Young modulus dimensioned as N/m, $\sigma_{zz}, \varepsilon_{zz}$ designate longitudinal components of stresses and surface strains.

Hence taking into account the surface effect allows obtaining a relation of effective elasticity modulus of a rod with pores E_S^* on a quantity of pores n. Moreover a small quantity of pores with a large area of cross-section weakens the rod (its stiffness becomes less than that of the rod made of isotropic material), however having the same total area of the pores' cross-section, a rod becomes the stiffer the more pores it contains (the less is radius of the pores).

4 A plane problem for a circular nanoscale hole in a plate (Kirsch problem)

Another problem, considered in this work and demonstrating that consideration of surface stresses has a significant impact on the mechanical properties of nanoobjects is a plane problem for a circular nanoscale hole.

Let's consider a respective problem of elasticity theory: an elastic plane with a circular cut with a radius R is under single-axis tension applied at infinity (Kirsch problem) of the value p and of additional surface stresses. Formulas for the surface [3, 4] and for bulk linear elasticity in the case of plane deformation give

$$\begin{aligned} &\sigma^S_{\varphi\varphi} = \sigma^S_0 + (\lambda_S + 2\mu_S)\varepsilon^S_{\varphi\varphi},\ \sigma^S_3 = \sigma^S_0 + \lambda_S \varepsilon^S_{\varphi\varphi}, \\ &\sigma_{\varphi\varphi} = (\lambda + 2\mu)\varepsilon_{\varphi\varphi} + \lambda\varepsilon_{rr},\ \sigma_{rr} = (\lambda + 2\mu)\varepsilon_{rr} + \lambda\varepsilon_{\varphi\varphi} \\ &\sigma_{r\varphi} = 2\mu\varepsilon_{r\varphi} + \lambda\varepsilon_{rr},\ \sigma_{33} = \lambda(\varepsilon_{rr} + \varepsilon_{\varphi\varphi}), \end{aligned} \tag{9}$$

Here (r,φ) is a polar coordinate system with the origin coinciding with the center of the cut, σ^S_0 is a residual surface stress corresponding to an unloaded body, $\sigma^S_{\varphi\varphi}$ and $\varepsilon^S_{\varphi\varphi}$ are circumferential surface stresses and strains, σ^S_{33} is a normal to surface tensor component of surface stresses, σ_{ij} and ε_{ij} are components of bulk stress and strain tensors, λ_S and μ_S are surface elastic moduli, analogous to Lamé parameters λ and μ for bulk isotropic elasticity.

Boundary conditions at the boundaries of the cut $r = R$ will be given as:

$$\sigma_{rr} - \frac{\sigma^S_{\varphi\varphi}}{R} = 0,\ \sigma_{r\varphi} + \frac{1}{R}\frac{\partial \sigma^S_{\varphi\varphi}}{\partial\varphi} = 0,$$

while the conditions at infinity in Cartesian coordinate system will be ($x_1 = r\cos\varphi$, $x_2 = r\sin\varphi$):

$$\lim_{r\to\infty}\omega = 0,\ \lim_{r\to\infty}\sigma_{ij} = 0,\ (i,j = 1,2),\ \text{exept}\ \lim_{r\to\infty}\sigma_{11} = p, \tag{10}$$

By solving the problem (9)-(10) using the method of complex functions we get for the exterior of the circle $r > R$ [11]

$$\begin{aligned} &\sigma_{rr}(r,\varphi) = \frac{\sigma^S_0}{R+M}\frac{R^2}{r^2} + \frac{p}{2}\left[1 - \left(1 - \frac{M(1+\kappa)}{2(R+M)}\right)\frac{R^2}{r^2} + \left(1 - \frac{4R^2}{r^2} + \left(3 - \frac{M(1+\kappa)}{2R+M(3+\kappa)}\right)\frac{R^4}{r^4}\right)\cos 2\varphi\right], \\ &\sigma_{\varphi\varphi}(r,\varphi) = -\frac{\sigma^S_0}{R+M}\frac{R^2}{r^2} + \frac{p}{2}\left[1 + \left(1 - \frac{M(1+\kappa)}{2(R+M)}\right)\frac{R^2}{r^2} - \left(1 + \left(3 - \frac{6M(1+\kappa)}{2R+M(3+\kappa)}\right)\frac{R^4}{r^4}\right)\cos 2\varphi\right], \\ &\sigma_{r\varphi}(r,\varphi) = -\frac{p}{2}\left[1 - 2\frac{R^2}{r^2} + \left(3 - \frac{4M(1+\kappa)}{2R+M(3+\kappa)}\right)\frac{R^4}{r^4}\right]\cos 2\varphi, \end{aligned} \tag{11}$$

with $M = (\lambda_S + 2\mu_S)/2\mu$, $\kappa = 3 - \nu$

Equalities (11) show a characteristic relation of stresses on the size of a nanoscale hole. Moreover, equalities (11) result in consideration of surface stresses decreases concentration of stresses in the vicinity of the cut if $M > 0$. An analogous effect is given by the remaining surface stress σ^S_0, that is actually a surface energy needed for creation of a surface unit. This is fair, for example, in the case of fcc metals $M \sim (10^{-10} - 10^{-9})m$, $\sigma^S_0 \sim 1N/m$ [5], and in this case the first summand in the second formula (11) obtains the order of $100MPa$ if the radius of the hole is $\alpha \sim 10nm$. This means that having stress values at infinity $p = 100MPa$, the input of the residual stresses σ^S_0 into strained state at the hole boundary is comparable to the input of a homogeneous strained state, which decreases significantly the concentration of stresses in the vicinity of the cut. This means in particular that a object with nanoscale cut is able to bear a significantly larger load till the moment of elasticity loss.

5 Stability of an infinite plate with a circular cut with consideration of surface effects

In fact energetic method introduced by S.P. Timoshenko can be applied in order to define the critical stress, when the loss of plane form of a plate occurs [13]:

$$\begin{aligned} &U = W, \\ &U = \tfrac{D}{2}\int_0^{2\pi}\int_R^{\infty}\left[(\Delta w)^2 - (1-\nu)L(w,w)\right] r dr d\varphi, \\ &W = \tfrac{h}{2}\int_0^{2\pi}\int_R^{\infty}\left[\sigma_{rr} r\left(\tfrac{\partial w}{\partial r}\right)^2 + \sigma_{\varphi\varphi}\tfrac{1}{r}\left(\tfrac{\partial w}{\partial \varphi}\right)^2 + 2\tau_{r\varphi} r \tfrac{\partial w}{\partial r}\tfrac{\partial w}{\partial \varphi})\right] dr d\varphi, \end{aligned} \tag{12}$$

where U is potential energy of bending strains,W is the work of the forces in a mid plane of the plate accumulated to the moment of stability loss on extra displacements, caused by buckling, w is deflection of a buckled plate, ν is the Poisson's ratio, $D = Eh^3/12(1-\nu)^2$ is a plate's cylindric stiffness, h is its stiffness,

$$L(w,w) = 2\left[\frac{1}{r}\frac{\partial^2 w}{\partial r^2}\frac{\partial w}{\partial r} + \frac{1}{r^2}\frac{\partial^2 w}{\partial \varphi^2}\frac{\partial w}{\partial r^2} - \frac{1}{r^2}\left(\frac{\partial^2 w}{\partial r \partial \varphi}\right)^2 + \frac{2}{r^3}\frac{\partial^2 w}{\partial r \partial \varphi}\frac{\partial w}{\partial \varphi} - \frac{1}{r^4}\left(\frac{\partial w}{\partial \varphi}\right)^2\right]$$

Searching for the function of deflection in the form$w(r,\varphi) = \sum_{i=1}^{3}\frac{a_i}{r^i}\cos\varphi$ and having coefficients a_i defined from the boundary conditions, we can obtain an expression for the critical load P_{cr} causing the stability loss, using the formula (20) and taking into consideration surface stresses at the hole.

In Table 1 critical loads P_{cr} are given in relation to critical loads in which surface stresses P_{cr_clas} are not taken into consideration for various thicknesses of the plate with the following parameters of the problem: $R = 15nm$, $E = 10^{11}N/m^2$, $\sigma_0^s = 1N/m$, $M = 5\cdot 10^{-9}m$, $\nu = 1/3$

Table 1.

h	0.5 nm	1 nm	10nm
P_{cr}/P_{cr_clas}	0.325	0.795	0.951

Hence taking surface stresses into consideration results in a significant increase of critical loads.

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