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On an approach to construction the basic of nanomaterials mechanics

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In the paper the basic relations for description of elastic deformation of nanoporous solids are proposed. They include a classical equilibrium equation and a constitutive relation between stress and strain tensors. While formulating the latter it is assumed that elastic moduli can be presented as a product of two functions. The first one depends on characteristic size of the nanoscale elements forming material, the second depends on the porosity coefficient. For description of the elastic moduli dependence on characteristic size the local gradient approach in thermomechanics is used. On the base of the model problems solutions for a layer and a cylinder there are investigated the nanoscale element geometry and size influences on elastic moduli, including Young modulus and Poisson coefficient.

Keywords: nanomaterials, local gradient approach, scale effect of elasticity moduli.

Introduction. Recently the scientific literature pays a considerable attention to the modeling, description and study of the properties of solids , distinguished by various size effects. Such solids feature comparable contributions of surface and volume factors to internal energy and one of their geometrical sizes (further — characteristic size) is comparable to the size of the region of nearsurface nonhomogeneity. The properties of the solids essentially differ from properties of solids without such effects. Structures of the nano-sized elements is a tool to create radically new devices and construction materials, also enabling to design and produce materials with the improved parameters [3, 4, 10, 14]. At present nano-elements and nanomaterials are widely used in electronics and nanobiotechnology.

Combining the nano-sized elements in an aggregate structure we get the material with a high degree of porosity [1, 4, 5] which further is called «nanomaterial». Porosity coefficient α is the fraction of the volume of an apparent solid that is actually an empty space (or filled with a foreign compound) and reaches 80 % or more in many cases. As a characteristic size of nanomaterial we understand the characteristic size r of nano-sized elements (see Fig. 1). It is obvious that mechanical properties of nano-porous solids depend not only on the porosity coefficient but also on the characteristic size of the nano-structure (parameter r). Porous materials, such as polymeric foams, metallic nano-sponge or fiber materials are widely used in practice. Lately, the composite reinforced by carbon nanotubes and nanofibres has been also widely used [4, 10].

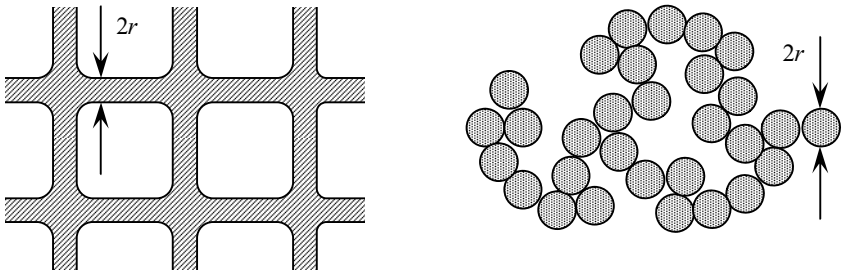

Fig. 1. Characteristic size of the nanostructures

For describing the mechanical behavior of nano-sized elements characterized by size effects, the various nonlocal models of mechanics are used. Usually the nonlocal dependence between tensors of strain and stress are postulated in such models [11, 12]. Such a dependence is often associated with characteristic size of a lattice, and also with the presence of defects in the solid [14]. Another approach allowing the description of various size effects in deformable solids is so called local gradient approach in thermomechanics [7, 8, 13]. This approach is based on basic relations of nonequilibrium thermodynamics and nonlinear mechanics. Within the framework of the approach the space of local state parameters is extended with chemical potential and its gradient. Thus, for local gradient elastic solid the state space consists of strain tensor $\hat{e}$, disturbance of chemical potential η and its gradient $\vec{\nabla}\eta$, and also coupled parameters: stress tensor $\hat{\sigma}$, density of mass ρ and elastic displacement of mass vector $\vec{\pi}_m$ [8]. It has been shown that chemical potential disturbance can be interpreted as disturbance of interaction energy. This opens a way to description of different conditions of particles interaction in the nearsurface and internal regions of the body.

The experimental study of nanomaterials is usually concentrated on investigation of physical-mechanical properties of a single nano-element, including dependence of elastic moduli on its characteristic size. Note that for determining the elastic moduli of thin porous layers the methods of surface acoustic wave spectroscopy, Brillouin light scattering, ellipsometric porosimetry, nanoindentation and others are used [2]. While investigating bionanomaterials an attention is concentrated on the study of corrosive, mutagen and carcinogen properties and also on methods of producing materials with physical and chemical properties similar to ones of bio tissues.

In this paper the basic relations of local gradient approach in thermomechanics are used for describing elastic deformation of nanoporous solids. The elastic moduli in constitutive relation between tensors of stress and strain are taken as a product of functions depending on the characteristic size of the nano-sized elements of material and porosity coefficient. The detailed study of Young modulus and Poisson coefficient is presented and the influence of geometry on the size effect is indicated.

1. Modeling of elastic properties of porous materials

The analysis of many theoretical and experimental researches allows us to assume that elastic deformable porous material can be described by the classic equations of motion (equilibrium) and the following governing relation

$$\hat{\sigma} = \frac{E}{1+\nu}\hat{e} + \frac{\nu E}{(1+\nu)(1-2\nu)} e\hat{I} \tag{1}$$

in which for Young modulus E and Poisson coefficient ν, is held

$$E = E_0 \varphi_E(\alpha), \qquad \nu = \nu_0 \varphi_\nu(\alpha). \tag{2}$$

Here $e = \hat{e} : \hat{I}$, $\hat{I}$ is identity tensor, α is porosity coefficient, φ_E, φ_ν are functions such that $\varphi_E(0) = \varphi_\nu(0) = 1, E_0, \nu_0$ are Young modulus and Poisson coefficient of a solid.

The exact presentation of functions φ_E, φ_ν is well described in scientific literature on the base of a wide experimental study. Usually in the literature there is a specified linear or near linear decrease of the Young modulus and nonlinear dependence of the shear modulus and Poisson coefficient for the growth of material porosity. In Fig. 2 the dependences of the Young modulus and Poisson coefficient on porosity α are presented in the region $0,4 \geq \alpha \geq 0$.

Let us use formulas (1), (2) to describe a porous nanomaterial. Thus it is necessary to accept that moduli E_0, ν_0 depend on a characteristic size of nanoelements on the basis of which the nanomaterial is constructed. For consideration of such dependences we will use local gradient approach in thermomechanics.

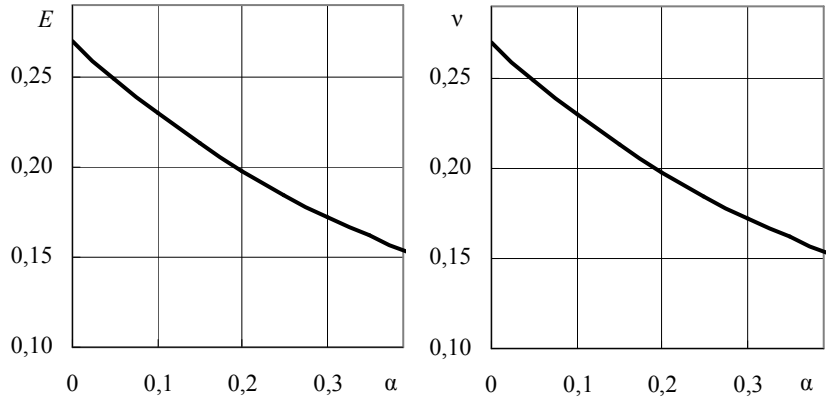

Fig. 2. Porosity α effect on Young modulus E (GN/m^2) and Poisson coefficient ν for iron [6]

2. Local gradient approach in thermomechanics and size effects of elasticity moduli

For local gradient approach in thermomechanics the state equations in the model of isotropic one-component elastic solid for linear approximation are the following [7]

$$\begin{aligned}
&\hat{\sigma} = 2a_{\mu}\hat{e} + \left(a_{\lambda}e + a_{eh}\eta\right)\hat{I}\,,\\
&\rho - \rho_{*} = -a_{eh}e - a_{hh}\eta\,,\\
&\vec{\pi}_{m} = -a_{gg}\vec{\nabla}\eta\,.
\end{aligned} \tag{3}$$

Here ρ^{*} is density of the solid material in the initial state, which is assumed to be the state of free of external loading homogeneous media with the material identical to material of the solid; a_{λ}, a_{μ}, a_{eh}, a_{gg}, a_{hh} are constants.

Note that taking as solving functions displacement vector $\vec{u}$ and chemical potential disturbance η the key equation set of the model for elastic solid state is

$$\begin{aligned}
&a_{\mu}\nabla^{2}\vec{u} + \left(a_{\mu} + a_{\lambda}\right)\vec{\nabla}\left(\vec{\nabla}\cdot\vec{u}\right) + a_{eh}\vec{\nabla}\eta = 0\,,\\
&a_{gg}\nabla^{2}\eta - a_{hh}\eta - a_{eh}\vec{\nabla}\cdot\vec{u} = 0\,.
\end{aligned}$$

If instead of displacement vector $\vec{u}$ the stress tensor is chosen as solving function the key equation set is

$$\begin{aligned}
&\vec{\nabla}\cdot\hat{\sigma} = 0\,,\\
&\vec{\nabla}\times\left[\left(3a_{\lambda} + 2a_{\mu}\right)\hat{\sigma} - \left(a_{\lambda}\sigma + 2a_{\mu}a_{eh}\eta\right)\hat{I}\right]\times\vec{\nabla} = 0\,,\\
&\nabla^{2}\eta - \kappa_{\eta}^{2}\eta - \kappa_{\sigma}^{2}\sigma = 0\,,
\end{aligned} \tag{4}$$

where $\kappa_{\eta}^{2} = \dfrac{1}{a_{gg}}\left(a_{hh} - \dfrac{3a_{eh}^{2}}{3a_{\lambda} + 2a_{\mu}}\right)$, $\kappa_{\sigma}^{2} = \dfrac{a_{eh}}{a_{gg}\left(3a_{\lambda} + 2a_{\mu}\right)}$, $\sigma = \hat{\sigma} : \hat{I}$.

For correct formulation of the problem these sets are to be supplemented with proper boundary condition.

In paper [9] on the base of solution of the model one-dimensional problem for layer $|x| \le l$ it is shown that local gradient approach allows describing the size effects (dependence on the layer thickness) of the elasticity moduli. For Young modulus E and Poisson coefficient ν it was

$$\begin{aligned}
&E = \left(3a_{\lambda} + 2a_{\mu}\right)\left[\frac{a_{\lambda} + a_{\mu}}{a_{\mu}} + \Psi\left(\xi l\right)\right]^{-1},\\
&\nu = \left(\frac{a_{\lambda}}{2a_{\mu}} - \Psi\left(\xi l\right)\right)\left[\frac{a_{\lambda} + a_{\mu}}{a_{\mu}} + \Psi\left(\xi l\right)\right]^{-1}.
\end{aligned} \tag{5}$$

Here $\xi^2=\kappa_\eta^2+b_m\kappa_\sigma^2$, $b_m=\dfrac{4a_\mu a_{eh}}{a_\lambda+2a_\mu}$, $\Psi(\xi l)=\dfrac{a_\lambda+2a_\mu}{4a_\mu}\dfrac{1-\zeta_l(\xi l)}{\zeta_l(\xi l)}$, $\zeta_l=1-D\left(1-\dfrac{\mathrm{th}(\xi l)}{\xi l}\right)$, $D=b_m\dfrac{\kappa_\sigma^2}{\xi^2}$. Let us note that parameter ξ^{-1} is characteristic size of the nearsurface non-homogeneity region.

For Lame constants λ, μ, shear G and bulk K moduli using formulas

$$\lambda=\frac{\nu E}{(1+\nu)(1-2\nu)},\quad \mu=G=\frac{E}{2(1+\nu)},\quad K=\frac{E}{3(1-2\nu)},$$

we write

$$\mu=G=a_\mu,$$
$$\lambda=\frac{a_\lambda-2a_\mu\Psi(\xi l)}{1+3\Psi(\xi l)},$$
$$K=\left(a_\lambda+\frac{2}{3}a_\mu\right)\Big/\left[1+3\Psi(\xi l)\right]. \qquad (6)$$

For layers of thickness satisfying relation $\exp(\xi l)>>1$ from (5), (6) maintaining moduli dependence on the layer thickness we get

$$E(\xi l)=E_\infty\left(1+\frac{b_E}{\xi l}\right),\quad \nu(\xi l)=\nu_\infty\left(1+\frac{b_\nu}{\xi l}\right),$$
$$\lambda(\xi l)=\lambda_\infty\left(1+\frac{\lambda_E}{\xi l}\right),\quad K(\xi l)=K_\infty\left(1+\frac{K_\nu}{\xi l}\right), \qquad (7)$$

where

$$E_\infty=\left(3a_\lambda+2a_\mu\right)\left(\frac{a_\lambda+a_\mu}{a_\mu}+\Psi_\infty\right)^{-1},\quad \nu_\infty=\left(\frac{a_\lambda}{2a_\mu}-\Psi_\infty\right)\left(\frac{a_\lambda+a_\mu}{a_\mu}+\Psi_\infty\right)^{-1},$$
$$\lambda_\infty=\frac{a_\lambda-2a_\mu\Psi_\infty}{1+3\Psi_\infty},\quad K_\infty=\frac{a_\lambda+2a_\mu/3}{1+3\Psi_\infty},\quad \Psi_\infty=\frac{a_\lambda+2a_\mu}{4a_\mu}\frac{D}{1-D},$$
$$b_E^{-1}=(1-D)\left(1+\frac{a_\lambda+a_\mu}{a_\mu\Psi_\infty}\right),\quad b_\nu=\frac{\Psi_\infty}{1-D}\left[\left(\frac{a_\lambda}{2a_\mu}-\Psi_\infty\right)^{-1}+\left(\frac{a_\lambda+a_\mu}{a_\mu}+\Psi_\infty\right)^{-1}\right],$$
$$b_\lambda=\frac{\left(3a_\lambda+2a_\mu\right)\Psi_\infty}{(1-D)\left(a_\lambda-2a_\mu\Psi_\infty\right)(1+3\Psi_\infty)},\quad b_K=\frac{3\Psi_\infty}{(1-D)(1+3\Psi_\infty)}.$$

From (7) it is easy to see that in the case of the characteristic size of the structure being far greater than the characteristic size of the nearsurface nonhomogeneity region

($\xi l >> 1$) we acquire $E = E_\infty$, $\nu = \nu_\infty$. In this case values of E_∞, ν_∞ can be interpreted as the elastic moduli specified for massive solids.

With the purpose of study of the surface curvature influence on the size effect of the elasticity moduli similar research was conducted for the solid cylinder of radius R. It was found, that dependence of the moduli on the radius R is described by formulas (5), (6), taking for function Ψ the expression

$$\Psi(\xi R) = \frac{a_\lambda + 2a_\mu}{4a_\mu} \frac{1 - \zeta_c(\xi R)}{\zeta_c(\xi R)}, \tag{8}$$

where $\zeta_c = 1 - D\left(1 - \dfrac{2I_1(\xi R)}{\xi R\, I_0(\xi R)}\right)$, I_0, I_1 are modified Bessel functions.

For accepted above approximation $\exp(\xi R) >> 1$ maintaining moduli dependence on the cylinder radius we obtain

$$E(\xi R) = E_\infty\left(1 + \frac{2b_E}{\xi R}\right), \quad \nu(\xi R) = \nu_\infty\left(1 + \frac{2b_\nu}{\xi R}\right),$$
$$\lambda(\xi R) = \lambda_\infty\left(1 + \frac{2b_\lambda}{\xi R}\right), \quad K(\xi R) = K_\infty\left(1 + \frac{2b_K}{\xi R}\right), \tag{9}$$

Comparing expressions of elasticity moduli obtained on the basis of solutions of model problems for a layer and a cylinder with same characteristic size $l = R$ we notice their dependence on the curvature. Such conclusion significantly differs from the basic position of classic mechanics of solids, when it is accepted, that the moduli are properties of material and do not depend on geometrical sizes and form of the body.

3. Constitutive relations for porous nanomaterials

Assume that the nanomaterial is porous and it is formed of the nanoelements with characteristic size r of elements forming nanomaterial. Therefore for its description we can use relations (1), (2), taking Young modulus E_0 and Poisson coefficient ν_0 depended on the size r. Thus we can write such determining relation

$$\hat{\sigma} = \frac{E_0(r)\varphi_E(\alpha)}{1 + \nu_0(r)\varphi_\nu(\alpha)}\hat{e} + \frac{\nu_0(r)E_0(r)\varphi_\nu(\alpha)\varphi_E(\alpha)}{[1 + \nu_0(r)\varphi_\nu(\alpha)][1 - 2\nu_0(r)\varphi_\nu(\alpha)]}e\hat{I}. \tag{10}$$

While studying the behavior of concrete bodies it is necessary to take into account the type of nanoelements that are used for forming the nanomaterial. In this case formula (8) must be specified using relations (5), (8) or (7), (9). The relation (10) together with the equilibrium equation forms a complete set of equations.

Conclusions. The approach to model description of the elastic deformation of deformable body made of nanomaterial is proposed. The complete equation set of the model includes classical equilibrium equation and stated constitutive equation relating tensors

of strain and stress. The latter is generalization of Hooke's law for porous material with account of the size effect of elastic moduli. The local gradient approach in thermomechanics is used for establishing the moduli dependences on a characteristic size of the nanostructure. The influence of geometry of elements forming nanomaterial on size effect is noted. The analysis of Young modulus and Poisson coefficient dependence on the characteristic size and geometry indicates that these moduli are the properties of concrete nanoelements (thin films, fibers etc). They become the properties of material for the solids with characteristic size far greater than the one of the region of nearsurface nonhomogeneity.

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Про підхід до побудови основ механіки наноматеріалів

Тарас Нагірний, Костянтин Червінка

У роботі запропоновано основні співвідношення для опису пружного деформування нанопористих тіл. Вони включають класичне рівняння рівноваги та визначальне співвідношення, що пов'язує тензори напружень і деформації. Під час формулювання останнього прийнято, що пружні модулі можна подати у вигляді добутку двох функцій. Перша із них залежить від характерного розміру наноелементів, що утворюють наноматеріал, тоді як друга — від коефіцієнта пористості. Для опису залежності пружних модулів від характерного розміру використано локально градієнтний підхід у термомеханіці. На основі модельних задач для шару та циліндра досліджено вплив геометрії та розміру наноелемента на величину пружних модулів матеріалу, включаючи модуль Юнга та коефіцієнт Пуассона.

О подходе к построению основ механики наноматериалов

Тарас Нагирный, Константин Червинка

В работе предложены основные соотношения для описания упругой деформации нанопористых тел. Они включают классическое уравнение равновесия и определяющее соотношение между тензорами напряжений и деформаций. При формулировке последнего принято, что упругие модули можно представить в виде произведения двух функций. Первая из них зависит от характерного размера наноелементов, образующих наноматериал, тогда как вторая — от коэффициента пористости. Для описания зависимости упругих модулей от характерного размера использован локально градиентный подход в термомеханике. На основе модельных задач для слоя и цилиндра исследовано влияние геометрии и размера наноелемента на величину упругих модулей материала, включая модуль Юнга и коэффициент Пуассона.

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