

To description of size effect of elastic moduli in electroconductive nonferromagnetic thin films

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The basic relations of the model of electroconductive nonferromagnetic solids taking into account the effects of local gradientality are presented. The size effect of elastic moduli, namely Young's modulus and Poisson's coefficient, is studied on the example of the stretched layer. It is shown that there are two specific sizes of the layer. The first is related to a nearsurface nonhomogeneity of interaction energy (chemical potential disturbance) and the second one — to Coulomb's interaction of the charged particles. The estimation of these parameters indicates that the first is far greater than the second one. With the layer thickness increase the elastic moduli tend to a constant value. Such investigations are important for constructing bases of mechanics of electroconductive nonferromagnetic nanomaterials.

Keywords: size effect of elasticity moduli, electroconductive thin films, local gradient approach.

Introduction. Considerable attention has been recently paid in scientific literature to studying, describing and modelling of the properties of solids, distinguished by various size effects. Such interest is caused, first of all, by the wide use in engineering practice of nanomaterials which are characterized by a commensurability of volume and surface factors in internal energy. Local gradient approach in thermomechanics [1, 2] is one of the effective approaches allowing to describe the near-surface non-homogeneity. In paper [3] within the framework of this approach on an example of the modelling problem for an electroconductive nonferromagnetic layer it is shown that two characteristic sizes are peculiar to the near-surface non-homogeneity. One of them is connected with solid particles interaction energy whereas the second one is connected with Coulomb's interaction of the charged particles. It must be noted that in the paper [3] the size effect of the ultimate stress limit (size effect of strength) of an electroconductive nonferromagnetic thin film has been studied and attention has been paid to its two scales. Note that in the literature the study of size effects of the elastic moduli is a subject of many works. Among them [4-6].

In this paper the basic relations of local gradient approach in thermomechanics are used for studying the size effect of the elastic modulus of electroconductive nonferromagnetic thin films. Such research is important, in particular, for construction of the bases of continual theory of mechanics of nanomaterials. The general approach to construction of such a theory is presented in [7].

1. Basic relations of local gradient mechanics of electroconductive nonferromagnetic solids

Let us suppose that the total energy E is expressed as a sum of internal U , kinetic K , and electromagnetic field U_e energies

$$E = U + K + U_e, \quad (1)$$

where the latter depends on the intensities of electric \vec{E} and magnetic \vec{H} fields

$$U_e = \frac{1}{2}(\varepsilon_0 \vec{E}^2 + \mu_0 \vec{H}^2), \quad (2)$$

and satisfies the equation of electromagnetic field balance

$$\frac{\partial U_e}{\partial \tau} = \frac{1}{\mu_0} \vec{\nabla} \cdot (\vec{E} \times \vec{B}) + (\vec{J}_\omega + \omega \vec{v}) \cdot \vec{E}.$$

Here τ is time, $\vec{B} = \mu_0 \vec{H}$, \vec{J}_ω is the vector of electric charge flux, ω is the electric charge density, \vec{v} is the barycentric velocity and ε_0, μ_0 are electric and magnetic constants.

The balance equation for the total energy under geometric linear approach is written in the form

$$\frac{\partial E}{\partial \tau} = \vec{\nabla} \cdot \left(\hat{\sigma} \cdot \vec{v} - T \vec{J}_s - H \vec{J}_m - \Phi \vec{J}_\omega + \frac{1}{\mu_0} \vec{E} \times \vec{B} \right). \quad (3)$$

Here $\hat{\sigma}$ is Cauchy stress tensor, T is temperature, H is chemical and Φ is thermodynamic electric potentials, \vec{J}_s and \vec{J}_m are the vectors of entropy and mass fluxes.

According to the local gradient approach in thermomechanics for thermodynamic fluxes it is assumed

$$\vec{J}_s = \vec{j}_s, \quad \vec{J}_\omega = -\frac{\partial \bar{\pi}_\omega}{\partial \tau} + \vec{j}_\omega, \quad \vec{J}_m = -\frac{\partial \bar{\pi}_m}{\partial \tau}, \quad (4)$$

where $\vec{j}_s, \vec{j}_\omega$ are irreversible components of fluxes $\vec{J}_s, \vec{J}_\omega$, and $\bar{\pi}_\omega, \bar{\pi}_m$ are vectors of reversible displacements of charge and mass, respectively.

Accepting a balance equation for momentum, entropy, mass and charge as follows

$$\begin{aligned} \frac{\partial \vec{k}_v}{\partial \tau} &= \vec{\nabla} \cdot \hat{\sigma} + \vec{F}_e, & \frac{\partial S}{\partial \tau} &= -\vec{\nabla} \cdot \vec{j}_s + \sigma_s, \\ \frac{\partial}{\partial \tau}(\rho - \vec{\nabla} \cdot \bar{\pi}_m) &= 0, & \frac{\partial}{\partial \tau}(\omega - \vec{\nabla} \cdot \bar{\pi}_\omega) &= -\vec{\nabla} \cdot \vec{j}_\omega \end{aligned} \quad (5)$$

and expression for kinetic energy change

$$\frac{\partial K}{\partial \tau} = \vec{v} \cdot \frac{\partial \vec{k}_v}{\partial \tau}, \quad (6)$$

relation (3) can be written as

$$\begin{aligned} \frac{\partial U}{\partial \tau} = & T \frac{\partial S}{\partial \tau} + H \frac{\partial \rho}{\partial \tau} + \Phi \frac{\partial \omega}{\partial \tau} + \hat{\sigma} : \frac{\partial \hat{e}}{\partial \tau} + \vec{\nabla} H \cdot \frac{\partial \vec{\pi}_m}{\partial \tau} + (\vec{\nabla} \Phi - \vec{E}') \cdot \frac{\partial \vec{\pi}_\omega}{\partial \tau} - \\ & - T \sigma_s - \vec{\nabla} T \cdot \vec{j}_s - (\vec{\nabla} \Phi - \vec{E}') \cdot \vec{j}_\omega. \end{aligned} \quad (7)$$

Here \vec{k}_v is linear mechanical motion momentum, $\vec{F}_e = (\vec{J}_\omega + \omega \vec{v}) \times \vec{B} + \omega \vec{E}$ is ponderomotive force, σ_s is entropy production, ρ is density of mass, $\vec{E}' = \vec{E} + \vec{v} \times \vec{B}$.

Note also that the third and the fourth equation of (5) become the classical equations of mass and charge balance when displacements are absent.

Formula (7) is a basis for formulation of the constitutive relations of the model. Taking into account that the dissipation energy $T \sigma_s$ is irreversibility measure and is characterised by thermodynamic fluxes on the base of Eq. (7) such a generalized Gibbs equation can be written

$$dU = TdS + Hd\rho + \Phi d\omega + \vec{\nabla} H \cdot d\vec{\pi}_m + (\vec{\nabla} \Phi - \vec{E}') \cdot d\vec{\pi}_\omega + \hat{\sigma} : d\hat{e}$$

as well as the expression for entropy production

$$\sigma_s = -\frac{1}{T} \vec{\nabla} T \cdot \vec{j}_s - \frac{1}{T} (\vec{\nabla} \Phi - \vec{E}') \cdot \vec{j}_\omega.$$

Introducing with Legendre transform

$$F = U - TS - H\rho - \Phi\omega - \vec{\nabla} H \cdot \vec{\pi}_m - (\vec{\nabla} \Phi - \vec{E}') \cdot \vec{\pi}_\omega$$

energy F , state equations are written as

$$\begin{aligned} S = -\frac{\partial F}{\partial T}, \quad \rho = -\frac{\partial F}{\partial H}, \quad \omega = -\frac{\partial F}{\partial \Phi}, \\ \vec{\pi}_m = -\frac{\partial F}{\partial (\vec{\nabla} H)}, \quad \vec{\pi}_\omega = -\frac{\partial F}{\partial (\vec{\nabla} \Phi - \vec{E}')}, \quad \hat{\sigma} = \frac{\partial F}{\partial \hat{e}}. \end{aligned}$$

The specific expressions of the state equations will be derived with concretization of energy F as a function of the state parameters $T, H, \Phi, \vec{\nabla} H, (\vec{\nabla} \Phi - \vec{E}'), \hat{e}$.

The key equation set of the electroconductive nonferromagnetic solid model written for solving functions $\hat{\sigma}, \eta, \Phi$ is

$$\begin{aligned} \vec{\nabla} \cdot \hat{\sigma} &= 0, \\ \vec{\nabla} \times \left\{ (3a_\lambda + 2a_\mu) \hat{\sigma} - [a_\lambda \sigma + 2a_\mu (a_{em} \eta + a_{e\omega} \Phi)] \hat{I} \right\} \times \vec{\nabla} &= 0, \\ \kappa_{mm} \nabla^2 \eta + \kappa_{m\omega} \nabla^2 \Phi - a_m \eta - a_\omega \Phi - a_\sigma \sigma &= 0, \\ \varepsilon_0 \nabla^2 \Phi + a_{m\omega} \eta + a_{\omega\omega} \Phi + a_{\sigma\omega} \sigma &= 0, \end{aligned} \quad (8)$$

where $\eta = H - H_*$ is chemical potential disturbance from the constant value H_* corresponding to the initial state (uniform infinite media of the material identical to those of the body); $\sigma = \hat{\sigma} : \hat{I}$; \hat{I} is identity tensor; $a_\lambda, a_\mu, a_{em}, a_{e\omega}, \kappa_{mm}, \kappa_{m\omega}, a_m, a_\omega, a_\sigma, a_{m\omega}, a_{\omega\omega}, a_{\sigma\omega}$ are constants.

2. State of a stretched electroconductive non-ferromagnetic thin film

Let us consider an isotropic electroconductive nonferromagnetic layer occupying region $|x| \leq l$ in Cartesian coordinates $\{x, y, z\}$. Assume that the values of chemical η_a and thermodynamic electric Φ_a potentials are given at the free of mechanical load surfaces $x = \pm l$. The layer is stretched at infinity $y \rightarrow \pm\infty$ with intensity σ_a . For such conditions one-dimensional situation is realized in the body.

Set (8) can be written in the form

$$\begin{aligned} \frac{d\sigma_{xx}}{dx} = 0, \quad \frac{d^2\sigma_{yy}}{dx^2} = \frac{d^2\sigma_{zz}}{dx^2}, \quad \frac{d^2}{dx^2}(\sigma - \beta_{\sigma\eta}\eta - \beta_{\sigma\Phi}\Phi) = 0, \\ \frac{d^2\eta}{dx^2} - \beta_{\eta\eta}\eta - \beta_{\eta\sigma}\sigma - \beta_{\eta\Phi}\Phi = 0, \quad \frac{d^2\Phi}{dx^2} - \beta_{\Phi\eta}\eta - \beta_{\Phi\sigma}\sigma - \beta_{\Phi\Phi}\Phi = 0. \end{aligned} \quad (9)$$

Here β_{ij} ($i, j = \eta, \sigma, \Phi$) are constants, expressed in terms of those given in (8):

$$\begin{aligned} \beta_{\sigma\eta} = 4a_\mu a_{em} / (a_\lambda + 2a_\mu), \quad \beta_{\sigma\Phi} = 4a_\mu a_{e\omega} / (a_\lambda + 2a_\mu), \quad \beta_{\Phi\eta} = -a_{m\omega} / \varepsilon_0, \\ \beta_{\Phi\sigma} = -a_{\sigma\omega} / \varepsilon_0, \quad \beta_{\Phi\Phi} = -a_{\omega\omega} / \varepsilon_0, \quad \beta_{\eta\eta} = \kappa_{mm}^{-1} (a_m + \kappa_{m\omega} a_{m\omega} / \varepsilon_0), \\ \beta_{\eta\sigma} = \kappa_{mm}^{-1} (a_\sigma + \kappa_{m\omega} a_{\sigma\omega} / \varepsilon_0), \quad \beta_{\eta\Phi} = \kappa_{mm}^{-1} (a_\omega + \kappa_{m\omega} a_{\omega\omega} / \varepsilon_0). \end{aligned}$$

Accept the boundary conditions at surfaces in the form

$$\vec{n} \cdot \hat{\sigma} = 0, \quad \eta = \eta_a, \quad \Phi = \Phi_a \quad (10)$$

and add integral conditions of mechanical force load of the body

$$\int_{-l}^l \sigma_{yy} dx = 2l\sigma_a, \quad \int_{-l}^l \sigma_{zz} dx = 0, \quad \int_{-l}^l x\sigma_{yy} dx = 0, \quad \int_{-l}^l x\sigma_{zz} dx = 0, \quad (11)$$

that correspond to uniaxial stretching ($\sigma_a > 0$) mechanical load.

Problems (9)-(11) solution can be written in the form

$$\begin{aligned} \eta - \eta_a = A_1 \left(\frac{\text{ch } \xi_1 x}{\text{ch } \xi_1 l} - 1 \right) + A_2 \left(\frac{\text{ch } \xi_2 x}{\text{ch } \xi_2 l} - 1 \right), \\ \Phi - \Phi_a = \frac{\xi_1^2 - a^2}{b^2} A_1 \left(\frac{\text{ch } \xi_1 x}{\text{ch } \xi_1 l} - 1 \right) + \frac{\xi_2^2 - a^2}{b^2} A_2 \left(\frac{\text{ch } \xi_2 x}{\text{ch } \xi_2 l} - 1 \right), \end{aligned}$$

$$\begin{aligned}\sigma - \sigma_a &= \sum_{k=1}^2 \left(\beta_{\sigma\eta} + \beta_{\sigma\varphi} \frac{\xi_k^2 - a^2}{b^2} \right) A_k \left(\frac{\operatorname{ch} \xi_k x}{\operatorname{ch} \xi_k l} - \frac{\operatorname{th} \xi_k l}{\xi_k l} \right), \\ \sigma_{,yy} - \sigma_a &= \sigma_{,zz} = \frac{1}{2} (\sigma - \sigma_a), \quad \sigma_{,xx} = 0.\end{aligned}\quad (12)$$

Here $a^2 = \beta_{\eta\eta} + \beta_{\sigma\eta}\beta_{\eta\sigma}$, $b^2 = \beta_{\eta\varphi} + \beta_{\sigma\varphi}\beta_{\eta\sigma}$, $c^2 = \beta_{\varphi\eta} + \beta_{\sigma\eta}\beta_{\varphi\sigma}$, $d^2 = \beta_{\varphi\varphi} + \beta_{\sigma\varphi}\beta_{\varphi\sigma}$;

$$\begin{aligned}A_k &= \frac{(-1)^{k-1}}{\Delta} \left\{ \frac{\beta_{\eta\eta}\eta_a + \beta_{\eta\varphi}\Phi_a + \beta_{\eta\sigma}\sigma_a}{a^2} \left[\chi_{c(3-k)} + \left(\xi_{3-k}^2 / d^2 - 1 \right)^{-1} \chi_{d(3-k)} \right] - \right. \\ &\quad \left. - \frac{\beta_{\varphi\eta}\eta_a + \beta_{\varphi\varphi}\Phi_a + \beta_{\varphi\sigma}\sigma_a}{c^2} \left[\chi_{ak} + \left(\xi_k^2 / a^2 - 1 \right) \chi_{bk} \right] \right\}, \quad k = 1, 2;\end{aligned}$$

$$\begin{aligned}\Delta &= \left[\chi_{a1} + \left(\xi_1^2 / a^2 - 1 \right) \chi_{b1} \right] \left[\chi_{c2} + \left(\xi_2^2 / d^2 - 1 \right)^{-1} \chi_{d2} \right] - \\ &\quad - \left[\chi_{a2} + \left(\xi_2^2 / a^2 - 1 \right) \chi_{b2} \right] \left[\chi_{c1} + \left(\xi_1^2 / d^2 - 1 \right)^{-1} \chi_{d1} \right];\end{aligned}$$

$$\chi_{tk} = 1 - D_t \left(1 - \frac{\operatorname{th} \xi_k l}{\xi_k l} \right), \quad t = a, b, c, d; \quad k = 1, 2;$$

$$D_a = \frac{\beta_{\sigma\eta}\beta_{\eta\sigma}}{a^2}, \quad D_b = \frac{\beta_{\sigma\varphi}\beta_{\eta\sigma}}{b^2}, \quad D_c = \frac{\beta_{\sigma\eta}\beta_{\varphi\sigma}}{c^2}, \quad D_d = \frac{\beta_{\sigma\varphi}\beta_{\varphi\sigma}}{d^2};$$

ξ_1, ξ_2 are the positive roots of equation $(\xi^2 - a^2)(\xi^2 - d^2) = b^2 c^2$.

The above relations describe the state of a thin electroconductive nonferromagnetic film with account of nearsurface nonhomogeneity effects. An analysis of the relations elicits existence of two specific sizes of nearsurface nonhomogeneity region. The first one, namely ξ_1^{-1} , is related to the nearsurface nonhomogeneity of interaction energy (chemical potential disturbance) and the second (ξ_2^{-1}) — to Coulomb's interaction of the charged particles. The performed estimation of these parameters indicates that $\xi_1^{-1} \gg \xi_2^{-1}$.

The stresses distribution in the considered body is analogous to that in the elastic layer [3]. For the considered external force load $\sigma_a > 0$ the greatest stresses in the film are surface stresses

$$\sigma_{,yy}(\pm l) = \sigma_a + \sum_{k=1}^2 \frac{A_k}{2} \left(\beta_{\sigma\eta} + \beta_{\sigma\varphi} \frac{\xi_k^2 - a^2}{b^2} \right) \left(1 - \frac{\operatorname{th} \xi_k l}{\xi_k l} \right).$$

These relations may be used for investigation of the strength parameters of the considered film. The investigation technique is presented in [8-10] and illustrated on the examples of elastic, thermoelastic thin films, fibres and solid solutions.

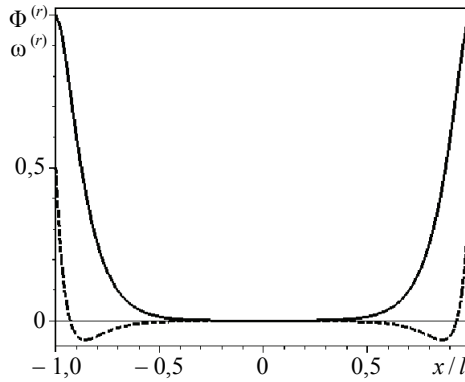


Fig. 1. Electric potential and charge distribution in the layer

Using state equations on the base of solution (12) the relations describing distributions of coupled state parameters can be written: densities of mass and charge as well as strain components. In Fig. 1 the electric potential and charge distribution in the layer, neglecting the stress influence on chemical and electric potentials, is presented.

3. Size effects of elastic moduli in the film

For investigation of the size effect of the elastic moduli, namely Young's modulus and Poisson's coefficient, we use their definition, that for a considered case can be written in the form

$$E = \frac{\sigma_a}{e_{yy}^0}, \quad \nu = -\frac{e_{xx}^0}{e_{yy}^0}, \quad (13)$$

where e_{yy}^0 , e_{xx}^0 are film strain compounds initiated by load σ_a only

$$e_{yy}^0 = e_{yy}|_{\sigma_a > 0} - e_{yy}|_{\sigma_a = 0}, \quad e_{xx}^0 = \frac{1}{2l} \int_{-l}^l (e_{xx}|_{\sigma_a > 0} - e_{xx}|_{\sigma_a = 0}) dx.$$

Obtaining from the state relation

$$\hat{\sigma} = 2a_\mu \hat{e} + (a_\lambda e + a_{em} \eta + a_{e\omega} \Phi) \hat{I},$$

strain components

$$\hat{e} = \frac{\hat{\sigma}}{2a_\mu} - \left[\frac{a_\lambda \sigma}{2a_\mu (3a_\lambda + 2a_\mu)} + \frac{a_{em} \eta + a_{e\omega} \Phi}{3a_\lambda + 2a_\mu} \right] \hat{I},$$

on the base of solution (12) and applying definition (13) we write

$$E = E_0 f_E(\xi_1 l, \xi_2 l), \quad \nu = \nu_0 f_\nu(\xi_1 l, \xi_2 l), \quad (14)$$

where

$$E_0 = \frac{a_\mu (3a_\lambda + 2a_\mu)}{a_\lambda + a_\mu}, \quad \nu_0 = \frac{a_\lambda}{2(a_\lambda + a_\mu)}, \quad f_E(\xi_1 l, \xi_2 l) = \left(1 + \frac{a_\lambda + 2a_\mu}{4(a_\lambda + a_\mu)} \Psi \right)^{-1},$$

$$f_\nu(\xi_1 l, \xi_2 l) = \left(1 - \frac{a_\lambda + 2a_\mu}{2a_\lambda} \Psi \right) / \left(1 + \frac{a_\lambda + 2a_\mu}{4(a_\lambda + a_\mu)} \Psi \right),$$

$$\Psi = \frac{1}{\Delta} \left\langle -2\Delta + \sum_{k=1}^2 (-1)^{k-1} \left\{ \left[\chi_{ak} + \chi_{bk} \left(\frac{\xi_k^2}{a^2} - 1 \right) \right] \left[1 + \left(\frac{\xi_{3-k}^2}{d^2} - 1 \right)^{-1} \right] - \left[\chi_{ck} + \chi_{dk} \left(\frac{\xi_k^2}{d^2} - 1 \right)^{-1} \right] \frac{\xi_{3-k}^2}{a^2} \right\} \right\rangle.$$

The Young's modulus E/E_0 dependence on the layer thickness $\xi_1 l$ for parameters $a_\lambda/a_\mu = 1; \xi_1/\xi_2 = 0, 2; D_a = 0,03; D_b = 0,05; D_3 = 0,05; D_d = 0,01; \xi_1/a = 0,75; \xi_1/d = 0,21$ (top curve), $D_a = 0,12, D_b = 0,14, D_3 = 0,14, D_d = 0,06, \xi_1/a = 0,50, \xi_1/d = 0,25$ (bottom curve) is illustrated in Fig. 2.

In scientific literature next to the moduli E, ν the Lamé parameters λ, μ , shear G and bulk K moduli are used. For Lamé 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

$$\mu = G = a_\mu,$$

$$\lambda = a_\lambda \left(1 - \frac{a_\lambda + 2a_\mu}{2a_\lambda} \Psi \right) / \left(1 + \frac{3(a_\lambda + 2a_\mu)}{4a_\mu} \Psi \right),$$

$$K = \left(a_\lambda + \frac{2a_\mu}{3} \right) / \left(1 + \frac{3(a_\lambda + 2a_\mu)}{4a_\mu} \Psi \right).$$

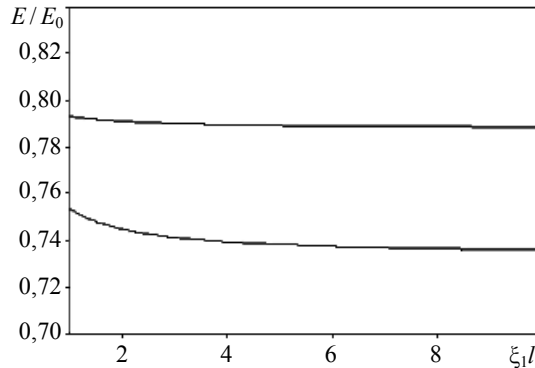


Fig. 2. Related Young's modulus change with the layer size increase

Conclusions. For the local gradient approach the basic model relations and key equation set for an electroconductive nonferromagnetic solid are presented and used to investigate the state of the uniaxial stretched layer, that models a thin film. On this basis the size effect of the elastic moduli, namely Young's modulus and Poisson's coefficient, is studied. It is shown that there are two specific sizes of the film. The first one is related to the nearsurface nonhomogeneity of interaction energy and the second is related to Coulomb's interaction of the charged particles. The estimation of these parameters indicates that the first parameter is far greater than the second one. With the layer thickness increase the elastic moduli tend to a constant value. The expressions for other elasticity moduli, namely Lamé constants, shear and bulk moduli, dependences on a characteristic sizes of the thin film are presented.

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До опису розмірного ефекту модулів пружності у електропровідних неферомагнітних тонких плівках

Тарас Нагірний, Костянтин Червінка

Подано основні співвідношення моделі електропровідного неферомагнітного твердого тіла з урахуванням ефектів локальної градієнтності. На прикладі розтягнутого шару досліджено розмірний ефект модулів пружності, а саме, модуля Юнга та коефіцієнта Пуассона. Вказано на два характерних розміри шару, перший із яких пов'язаний із приповерхневою неоднорідністю енергії взаємодії (збурення хімічного потенціалу), а другий — із кулонівською взаємодією заряджених частинок. Оцінка цих параметрів вказує, що перший є значно більший від другого. Із зростанням товщини шару модулі пружності прямують до усталеного значення. Проведені дослідження є важливі під час побудови основ механіки електропровідних неферомагнітних наноматеріалів.

К описанию размерного эффекта модулей упругости в электропроводных неферромагнитных тонких пленках

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Представлены основные соотношения модели электропроводного неферромагнитного твердого тела с учетом эффектов локальной градиентности. На примере растянутого слоя исследован размерный эффект модулей упругости, а именно, модуля Юнга и коэффициента Пуассона. Указано на два характерных размера слоя, первый из которых связан с приповерхностной неоднородностью энергии взаимодействия (возмущения химического потенциала), а второй — с кулоновским взаимодействием заряженных частиц. Оценка этих параметров указывает, что первый является значительно большим от второго. С ростом толщины слоя модули упругости стремятся к постоянной величине. Проведенные исследования являются важными при построении основ механики электропроводных неферромагнитных наноматериалов.

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