M$^{\text{odeling}}$ M C$^{\text{omputing}}$ athematical

Stress-deformed state and strength of a locally heterogeneous electrically conductive layer

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The key system of equations of the solid body model is presented, taking into account the structural heterogeneity of the material and the roughness of the real surface, which is applied to the study of interconnected fields in an unbounded heterogeneous conductive layer. The effect of taking into account the dependences on the density of local Young's modulus and Poisson's ratio on the size effects of surface stresses in the layer and its strength limit is considered.

1. Introduction

Determining the deformation and strength parameters of solid bodies is based on the problems of solid medium mechanics, which describe interconnected physical processes in the studied bodies. The basis of such studies is the use of appropriate models of physical and mechanical processes in bodies, which take into account local variations in density and elastic properties of the material [1, 2].

The technique involving the application of mass sources for modeling surface roughness is proposed in [3–5]. In works [6, 7] the key systems of equations of the mathematical model of a locally inhomogeneous electrically conductive non-ferromagnetic solid with consideration of the size effect were formulated, and the corresponding boundary conditions for the mass density distribution were substantiated in [8, 9]. Since all mechanical properties (density, elasticity, and others) are determined by the state of the spatial structure of the material of the body [10], a natural extension of the model is to take into account the heterogeneity of the modulus of elasticity [2]. In [11], an approach to the description of heterogeneous elastic bodies, whose elastic moduli depend on the local density of the mass, but without taking into account the electrical conductivity of the body, is proposed. According to [12], consideration of the electric field is essential when describing deformable conductive bodies, and local changes in density may be the cause of its uneven distribution.

This work presents a study of the stress-strain state of a structurally heterogeneous, electrically conductive, non-ferromagnetic solid, taking into account the dependence of the modulus of elasticity on the density. The strength of the stretched layer was studied and the size effects of surface stresses were investigated.

2. Statement of the problem

Let us consider an isotropic deformable electrically conductive, nonferromagnetic electroneutral solid layer occupying an area in a rectangular Cartesian coordinate system. Such a system is the subject of research both in quantum physics [13–15], as well as in the classical one [2], as it is a model of various

substrates, films that are widely used in nanotechnology, and which is characterized by the so-called size effect, that is, the dependence of some characteristics of the layer on its thickness.

We consider that the surfaces of the layer are free from external force load and a constant density value is set on them, different from the reference value, which is characteristic of an infinite medium. At infinity, the layer is loaded with tensile forces of intensity in the direction of the axis.

Under such a statement, the solving functions will depend only on the coordinate. We write the solving system of equations in terms of density, electric potential, and components of the stress tensor. For non-zero key functions, the system of equations of the model, neglecting the effect of stresses on the distribution of the electric potential according to [2, 7], is as follows:

$$
\begin{aligned}
&\frac{d\sigma_{xx}}{dx} = 0, \\
&\frac{d^2}{dx^2}\left(\frac{1+\nu}{E}\sigma_{yy} - \frac{\nu}{E}\sigma\right) = -\frac{d^2}{dx^2}\left[a_m\left(\rho - \rho_*\right) + a_0^\omega \phi\right], \\
&\frac{d^2}{dx^2}\left(\frac{1+\nu}{E}\sigma_{zz} - \frac{\nu}{E}\sigma\right) = -\frac{d^2}{dx^2}\left[a_m\left(\rho - \rho_*\right) + a_0^\omega \phi\right], \\
&\frac{d^2\rho}{dx^2} - \xi^2\left(\rho - \rho_*\right) = -\xi^2 d_{\sigma m}, \\
&\varepsilon_0 \frac{d^2\phi}{dx^2} + a_{\omega\omega}\phi + a_{m\omega}\left(\rho - \rho_*\right) = 0.
\end{aligned}
\tag{1}
$$

Here $\sigma = \sigma_{xx} + \sigma_{yy} + \sigma_{zz}$ is the spherical component of the stress tensor, σ_{xx}, σ_{yy}, σ_{zz} are nonzero components of the stress tensor, a_m, a_0^ω, ξ, ε_0, $a_{\omega\omega}$, $a_{m\omega}$ are constants, E, ν are Young's modulus and Poisson's ratio of the body material, $d_{\sigma m}$ is the intensity of the mass sources determined by the ratio

$$
d_{\sigma m} = (\rho_a - \rho_*)\frac{\cosh(\zeta x)}{\cosh(\zeta \ell)}.
\tag{2}
$$

The present parameter ζ, characterizing the distribution of mass sources is related to the geometric heterogeneity of the body surface and depends on the methods of its formation.

At the same time, we accept the dependence of the modulus of elasticity on the density [11]

$$
E = E_0\left(\frac{\rho}{\rho_*}\right)^{\beta_e}, \quad \nu = \nu_0\left(\frac{\rho}{\rho_*}\right)^{\beta_n},
\tag{3}
$$

where E_0, ν_0 are Young's modulus and Poisson's ratio of the body material in the reference state, β_e, β_n are constants. We will add conditions to the system formulated above:

$$
\rho(\pm\ell) = \rho_a, \quad \Phi(\pm\ell) = \Phi_a, \quad \sigma_{xx}(\pm\ell) = 0,
$$

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

$$
\int_{-\ell}^{\ell} x\,\sigma_{yy}(x)dx = 0, \quad \int_{-\ell}^{\ell} x\,\sigma_{zz}(x)dx = 0.
\tag{4}
$$

Surface values of electric potential present here ϕ_a are determined from the condition of electroneutrality of the layer

$$
\int_{-\ell}^{\ell} \omega(x)dx = 0,
\tag{5}
$$

where the electric charge is determined by the following relation:

$$
\omega = -a_{\omega\omega}\phi - a_{m\omega}\left(\rho - \rho_*\right).
\tag{6}
$$

The presented problem in a nonlinear formulation can be considered as a continuation of similar studies for the case of a linear formulation of the problem with $\beta_e = \beta_n = 0$ [7], as well as an extension of the model presented in [2] to the case of an electrically conductive body.

3. Analysis of the problem solution

The analysis of problem (1)–(6) shows that it is possible to consistently determine the density $\rho(x)$, thermodynamic electric potential $\phi(x)$ and stresses $\sigma_{xx}(x)$, $\sigma_{yy}(x)$, $\sigma_{zz}(x)$. The solution of the formulated problem has the form

$$\rho(x) - \rho_* = \frac{1}{D}\left(\rho_a - \rho_*\right)\left(\frac{\cosh(\xi x)}{\cosh(\xi \ell)} - \frac{\xi^2}{\zeta^2}\frac{\cosh(\zeta x)}{\cosh(\zeta \ell)}\right), \tag{7}$$

$$\phi(x) = \alpha_\phi \frac{\rho_a - \rho_*}{D}\left[\frac{\chi^2}{\xi^2 - \chi^2}\frac{\cosh(\xi x)}{\cosh(\xi \ell)} - \frac{\chi^2}{\zeta^2 - \chi^2}\frac{\xi^2}{\zeta^2}\frac{\cosh(\zeta x)}{\cosh(\zeta \ell)} - \right.$$
$$\left. - \left(\frac{\chi^2}{\xi^2 - \chi^2}\frac{\xi\tanh(\xi\ell)}{\chi\tanh(\chi\ell)} - \frac{\chi^2}{\zeta^2 - \chi^2}\frac{\xi^2}{\zeta^2}\frac{\zeta\tanh(\zeta\ell)}{\chi\tanh(\chi\ell)}\right)\frac{\cosh(\chi x)}{\cosh(\chi\ell)}\right], \tag{8}$$

$$\sigma_{xx}(x) = 0,$$

$$\sigma_{yy}(x) = -\frac{E(x)a_m\rho_*}{1 - \nu(x)}\left[\frac{\rho(x)}{\rho_*} - 1 + a_1^\omega\frac{\phi(x)}{\rho_*} - \frac{In_1}{In_2}\right] + \frac{\sigma_a}{2E_0 In_2}\frac{E(x)}{1 + \nu(x)}\left(\frac{1 + \nu(x)}{1 - \nu(x)} + \frac{In_2}{In_0}\right),$$

$$\sigma_{zz}(x) = -\frac{E(x)a_m\rho_*}{1 - \nu(x)}\left[\frac{\rho(x)}{\rho_*} - 1 + a_1^\omega\frac{\phi(x)}{\rho_*} - \frac{In_1}{In_2}\right] + \frac{\sigma_a}{2E_0 In_2}\frac{E(x)}{1 + \nu(x)}\left(\frac{1 + \nu(x)}{1 - \nu(x)} - \frac{In_2}{In_0}\right), \tag{9}$$

here

$$D = \frac{\zeta^2 - \xi^2}{\zeta^2}, \quad \chi^2 = -\frac{a_{\omega\omega}}{\varepsilon_0}, \quad \alpha_\phi = \frac{a_{m\omega}}{a_{\omega\omega}}, \quad a_1^\omega = \frac{a_0^\omega}{a_m},$$

$$In_0 = \frac{1}{2\ell E_0}\int_{-\ell}^{\ell}\frac{E(t)dt}{1 + \nu(t)}, \quad In_1 = \frac{1}{2\ell E_0}\int_{-\ell}^{\ell}\frac{E(t)}{1 - \nu(t)}\left(\frac{\rho(t)}{\rho_*} - 1\right)dt, \quad In_2 = \frac{1}{2\ell E_0}\int_{-\ell}^{\ell}\frac{E(t)}{1 - \nu(t)}a_1^\omega\frac{\phi(t)}{\rho_*}dt.$$

In the above ratios, according to [2], the parameter χ related to the electronic subsystem of the body, and ξ^{-1} is the characteristic size of structural heterogeneity of the material and it is assumed that

$$\chi^{-1} \ll \xi^{-1}, \quad \chi^{-1} \ll \zeta^{-1}.$$

Due to the electroneutrality condition (5), the charge is self-equilibrated by the thickness of the layer. According to (6), taking into account (7) and (8) near the surfaces $x = \pm\ell$ layer, the value of the electric charge is negative, while in the inner regions of the layer it is positive, which is consistent with the theory of the electric double layer [16], in particular the Gui–Chapman model [17]

$$\Phi_a = -\alpha_\phi \frac{(\rho_a - \rho_*)}{D}\left(\frac{\chi}{\xi}\frac{\tanh(\xi l)}{\tanh(\chi l)} - \frac{\chi}{\zeta}\frac{\xi^2}{\zeta^2}\frac{\tanh(\zeta l)}{\tanh(\chi l)}\right)$$
$$- \alpha_\phi\frac{(\rho_a - \rho_*)}{D}\left[\frac{\chi^2}{(\xi^2 - \chi^2)}\left(\frac{\chi}{\xi}\frac{\tanh(\xi l)}{\tanh(\chi l)} - 1\right) - \frac{\xi^2}{\zeta^2}\frac{\chi^2}{(\zeta^2 - \chi^2)}\left(\frac{\chi}{\zeta}\frac{\tanh(\zeta l)}{\tanh(\chi l)} - 1\right)\right]. \tag{10}$$

It can be seen from relation (10) that the influence of the size of the body is insignificant, and as the thickness of the layer increases, the value of the thermodynamic electric potential on its surface approaches the value characteristic of the surface of a half-space [11].

In the case of structurally heterogeneous bodies, the stress state will depend both on the conditions of the force load of the body, which is determined by the parameter σ_a, and stresses caused by various conditions of interaction of particles near the surface of the body, which depend on the near-surface density perturbation $r = \frac{\rho_a}{\rho_*}$.

To study the stress distribution, we first consider the solution (9) under the condition $\sigma_a = 0$, and then we study the strength properties of the body on the example of a stretched layer ($\sigma_a > 0$).

Numerical studies of the stress state in the layer were carried out on the basis of the obtained solutions. In Fig. 1, it is shown the distribution of stresses in a structurally heterogeneous layer, taking into account the nonlinear dependence of elastic characteristics.

The calculations were carried out at the following values: $\rho_a/\rho_* = 0.5$, $\xi\ell = 6$, $\nu_0 = 0.33$, $\chi/\xi = 5$, $a_1^\omega\alpha_\phi = -0.4$, $\zeta/\xi = 1.2$.

In Fig. 1a, curves 1–4 correspond to the following selection of parameters: $\beta_e = \beta_n = 0$; $\beta_e = 1$, $\beta_n = 0$; $\beta_e = 0$, $\beta_n = 1$; $\beta_e = \beta_n = 1$. At $\zeta/\xi = 1.2$, $\beta_e = 1$, $\beta_n = 0$, the parameter χ/ξ change from 2.4
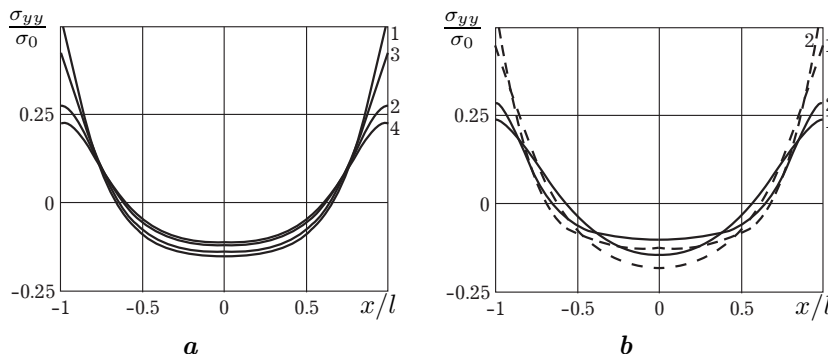

Fig. 1. Stress distribution in the layer.

to 24 gives a reduction of stresses in the center $x = 0$ layer, and when approaching the surface of the layer at $x = \pm l$ there is some increase in the amount of stress. In general, taking into account the dependence of local elastic moduli on density leads to a decrease in the surface stresses values.

The graph in Fig. 1b shows the stress distribution at $\zeta/\xi = 0.6$; 2.4 (curves 1–2), $\chi/\xi = 5$, $\xi l = 6$, $\rho_a/\rho_* = 0.5$, $a_1^\omega\alpha_\phi = -0.4$, $\nu_* = 0.33$. Solid lines correspond $\beta_e = \beta_n = 1$, and dotted — $\beta_e = \beta_n = 0$.

Analysis of the results of numerical studies shows that the distribution of stresses is symmetrical across the thickness of the layer, near-surface stresses are tensile, and in the middle part of the layer — compressive. Taking into account the dependence of the Young's modulus on the density leads to a decrease in surface tension compared to the case of a linear formulation of the problem $\beta_e = \beta_n = 0$ [2, 18].

In Fig. 2 illustrates the dependence of surface stresses on parameters β_e, β_n.

On the graph, curves 1–3 correspond to $\xi\ell = 3$; 6; 20 and built at $\rho_a/\rho_* = 0.5$, $a_1^\omega\alpha_\varphi = -0.4$, $\nu_0 = 0.33$, $\chi/\xi = 5$, $\zeta/\xi = 1.2$. The curves in Fig. 2a are constructed at $\beta_n = 0$, and in Fig. 2b at $\beta_e = 0$.
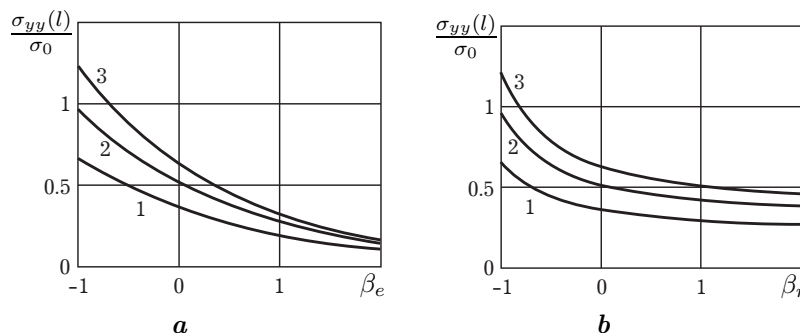
As the analysis of Figs. 1, 2 shows, nonlinearity parameters have the most significant effect on surface stresses.

Fig. 2. Dependence of surface stresses on parameters β_e, β_n.

4. Size effect of the layer strength limit

In order to assess the strength of the layer, we will use the method given in works [2, 11]. For tensile surface stresses, as shown in previous studies, which are the largest in the body, on the basis of (9) we write

$$\sigma_{yy}(\pm\ell) = -\sigma_0 \frac{(1-\nu_0)r^{\beta_e}}{1-\nu_0 r^{\beta_n}}\left[r - 1 + a_1^\omega\frac{\phi_a}{\rho_*} - \frac{In_1}{In_2}\right] + \frac{\sigma_a}{2In_2}\frac{r^{\beta_e}}{1+\nu_0 r^{\beta_n}}\left(\frac{1+\nu_0 r^{\beta_n}}{1-\nu_0 r^{\beta_n}} + \frac{In_2}{In_0}\right), \quad (11)$$

where $\sigma_0 = \frac{E_0\rho_* a_m}{(1-\nu_0)}$, $r = \frac{\rho_a}{\rho_*}$ are parameters.

Introduce the notation

$$A = \frac{1}{2In_2}\frac{r^{\beta_e}}{1+\nu_0 r^{\beta_n}}\left(\frac{1+\nu_0 r^{\beta_n}}{1-\nu_0 r^{\beta_n}} + \frac{In_2}{In_0}\right), \quad (12)$$

$$B = -\frac{(1-\nu_0)r^{\beta_e}}{1-\nu_0 r^{\beta_n}}\left[r - 1 + a_1^\omega\frac{\phi_a}{\rho_*} - \frac{In_1}{In_2}\right]$$

we write the relation (11) as follows

$$\sigma_{yy}(\pm\ell) = A\sigma_a + B\sigma_0.$$

Let us determine the intensity of the force load, which will lead to the destruction of the layer. As the starting point, we choose the criterion of the first classical theory of strength [19], according to which the destruction of the material occurs when the principal stress is the largest (in this case σ_{yy}) reaches a critical value for the material of the body σ_p. From the condition $\sigma_{yy}(\pm\ell) = \sigma_p$ we find the value $\sigma_a > 0$, at which the layer is subjected to non-elastic deformations or destruction, and we denote it σ_{cr}

$$\sigma_{cr} = \frac{1}{A}\left(\sigma_p - B\sigma_0\right). \tag{13}$$

For intensity σ_+ force load, which leads to the destruction of a thick layer, we obtain

$$\sigma_+ = \frac{1}{A^\infty}\left(\sigma_p - B^\infty\sigma_0\right), \tag{14}$$

where

$$A^\infty = \lim_{l\to\infty} A, \quad B^\infty = \lim_{l\to\infty} B.$$

Given the designation σ_+, relation (14) is written as

$$\sigma_{cr} = \frac{1}{A}\big(A^\infty\sigma_+ + (B^\infty - B)\sigma_0\big). \tag{15}$$

We will note as In_0^∞, In_1^∞, In_2^∞ limit values, respectively, for In_0, In_1, In_2 at $\ell \to \infty$. Then we write the relation (15) as follows

$$\sigma_{cr} = \frac{In_2 In_0}{In_2^\infty In_0^\infty}\frac{In_0^\infty\left(1+\nu_0 r^{\beta_n}\right) + In_2^\infty\left(1-\nu_0 r^{\beta_n}\right)}{In_0\left(1+\nu_0 r^{\beta_n}\right) + In_2\left(1-\nu_0 r^{\beta_n}\right)}\sigma_+$$
$$+ \frac{2In_0}{In_2^\infty}\frac{\left(1+\nu_0 r^{\beta_n}\right)\left(1-\nu_0\right)\left(In_2 In_1^\infty - In_1 In_2^\infty\right)}{\left(In_0\left(1+\nu_0 r^{\beta_n}\right) + In_2\left(1-\nu_0 r^{\beta_n}\right)\right)}\sigma_0. \tag{16}$$

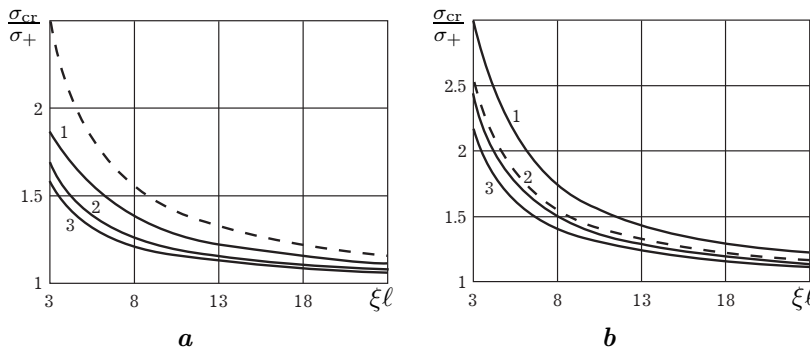In Fig. 3, it is shown the dependence of the critical load on the layer thickness.

In Fig. 3a shows the dependence of the reduced critical load σ_{cr}/σ_+ layer for $\rho_a/\rho_* = 0.5$, $\zeta/\xi = 0.6, 1.2, 2.4$ (curves 1–3), $\chi/\xi = 5$, $\nu_0 = 0.33$, $\beta_e = 1$, $\beta_n = 0$, $\sigma_0/\sigma_+ = 5$, $a_1^\omega\alpha_\phi = -0.4$. In Fig. 3b shows this dependence at $\beta_e = 0$, $\beta_n = 1$. Dashed curves in both figures correspond $\beta_e = \beta_n = 0$, excluding mass sources.

Fig. 3. The size effect of the critical layer load.

Comparing the values of the force load, which leads to the brittle destruction of the layer, obtained on the basis of the linearized model, when the dependence of the modulus of elasticity on the density is not taken into account, with the results obtained when such a dependence is taken into account, we see their significant quantitative difference, especially in the case of thin films.

The change of parameter χ/ξ does not significantly change the value σ_{cr}, and the electronic subsystem of the body affects the size effect of strength due to the parameter $a_1^\omega\alpha_\phi$, which in (11), (12) is included In_1, In_1^∞ linearly.

Therefore, expression (16) can be characterized as a ratio that describes the dependence of the strength limit on the electronic subsystem, as well as on the parameters of the structural heterogeneity of materials and the roughness of the real surface of the body and on its characteristic size.

5. Conclusions

On the basis of the conducted research, the following can be asserted.

— In a locally inhomogeneous electrically conductive non-ferromagnetic layer, free from external force loading, there is a non-zero stress-strain state and distributions of electric potential and charge, which should be taken into account when calculating the operational characteristics of the body.

— The influence of heterogeneity parameters on the stress-strain state of thin films can be investigated by taking into account the dependence of local elastic moduli on the variable density of the body. For the obtained nonlinear problem, the solution can be written in an explicit form.

— The values of thermodynamic electric potential and charge, which are established on the surface of the body, within the framework of the considered model, are uniquely determined by the physical and geometric parameters of the body. In turn, the value of the electric charge established on the surface of the body changes with a change in the ratio of characteristic sizes.

— The distribution of fields in the body is characterized by three characteristic sizes associated with Coulomb interaction forces, local heterogeneity of the body material, and geometric heterogeneity of the body surface.

— Surface stresses in the body are characterized by a three-scale Romer effect. Taking into account the non-linear representation of the modulus of elasticity when conducting numerical studies leads to a decrease in surface stresses in comparison with the linear formulation.

— Taking into account the nonlinearity of the Young's modulus significantly changes the value of the strength limit and affects its size effect, while the effect of the nonlinearity of the Poisson's ratio is much weaker. The strength of thin films increases as their thickness decreases.

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Напружено-деформований стан та міцність локально неоднорідного електропровідного шару

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Представлено ключову систему рівнянь моделі твердого тіла із врахуванням структурної неоднорідності матеріалу та шорсткості реальної поверхні, яку застосовано до вивчення взаємозв'язаних полів у необмеженому гетерогенному електропровідному шарі. Розглянуто вплив врахування залежностей від густини локальних модуля Юнга та коефіцієнта Пуассона на розмірні ефекти поверхневих напружень в шарі та межу його міцності.

Ключові слова: *електропровідне тіло, напруження, модулі пружності, розмірні ефекти, міцність.*