Effect of a Type of Loading on Stresses at a Planar Boundary of a Nanomaterial

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Abstract A two-dimensional model of an elastic body at nanoscale is considered as a half-plane under the action of a periodic load at the boundary. An additional surface stress, and constitutive equations of the Gurtin–Murdoch surface linear elasticity are assumed. Using Goursat–Kolosov complex potentials and Muskhelisvili technique, the solution of the boundary value problem in the case of an arbitrary load is reduced to a hypersingular integral equation in an unknown surface stress. For the case of a periodic load, the solution of this equation is found in the form of Fourier series. The influence of the surface stress on the stresses at the boundary of the half-plane under the tangential and normal periodic loading is analyzed. In particular, it is found out the size effect which becomes apparent in the dependence of the stresses on a length of the load period of the order 10 nm. Moreover, the tangential stresses appear under the action of the normal loads.

1 Introduction

The near-surface effects which are intrinsic to nanomaterials can cause an essential difference of physical properties of these nanomaterials from the same properties of macroscale bodies. Thus, physical properties of a nanometer specimen depend on its size (size effect). For example, Young's modulus of a cylindrical specimen increases significantly, when the cylinder diameter becomes very small [10].

As a rule, an ideal effect of a surface stress on the elastic body is not taken into account at the macroscale because it is insignificant in comparison with the

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effect of external forces. The Gurtin–Murdoch theory of surface elasticity which has obtained rapid development in recent years is extensively used to consider the surface properties of nanoobjects [1, 7].

In this paper the Gurtin-Murdoch model is applied to a semi-infinite linear elastic body with plane surface under plane strain conditions. The action of external forces at the boundary and surface stresses is assumed. Based on Goursat–Kolosove complex potentials and the Muskhelisvili approach, the boundary value problem is reduced to a hypersingular integral equation. The solution of this equation in the case of a periodic loading is used to analyze an influence of the surface stress on the stress state of the boundary in relation to a change of the period and type of loading.

2 Basic Equations

Consider the elastic half-space its surface has elastic properties differing from those in the bulk material. We assume that the media is in conditions of plane strain under the action of an external surface load and the additional surface stress. Thus, we come to the formulation of the boundary value problem for the half-plane $\Omega = \{z : \operatorname{Im} z < 0,\ \operatorname{Re} z \in \mathbb{R}^1\},\ z = x_1 + ix_3$,with the rectilinear boundary Γ.

In general case, the boundary condition is described by generalized Young–Laplace law [7]

$$\mathbf{n} \cdot \boldsymbol{\Sigma} - \nabla_s \cdot \boldsymbol{\tau} = \mathbf{p}, \tag{1}$$

where $\mathbf{n}$ is the unit vector normal to the boundary surface, $\boldsymbol{\Sigma}$ is the tensor of volume stress, $\boldsymbol{\tau}$ is the tensor of surface stress, $\mathbf{p}$ is the vector of an external surface load. Equation (1) means that the action of the surface stress is replaced by the corresponding load $\mathbf{t}_s(z) = \nabla_s \boldsymbol{\tau}$ defined by the surface gradient operator $\nabla_s = \nabla - \mathbf{n}\partial/\partial n$, where ∇ is the Hamilton operator [2]

$$\mathbf{t}_s(z) = -\left(\frac{\tau_{11}}{R_1} + \frac{\tau_{22}}{R_2}\right)\mathbf{n} + \frac{\mathbf{e}_1}{h_1 h_2}\left(\frac{\partial}{\partial \alpha_1}(h_2\tau_{11}) + \frac{\partial}{\partial \alpha_2}(h_1\tau_{21}) + \frac{\partial h_1}{\partial \alpha_2}\tau_{12} - \frac{\partial h_2}{\partial \alpha_1}\tau_{22}\right)$$
$$+ \frac{\mathbf{e}_2}{h_1 h_2}\left(-\frac{\partial h_1}{\partial \alpha_2}\tau_{11} + \frac{\partial}{\partial \alpha_1}(h_2\tau_{12}) + \frac{\partial h_2}{\partial \alpha_1}\tau_{21} + \frac{\partial}{\partial \alpha_2}(h_1\tau_{22})\right) \tag{2}$$

Here $\mathbf{e}_1$, $\mathbf{e}_2$ are the basis vectors of a curvilinear coordinate system α_1 and α_2; h_1, h_2 are the corresponding metric factors, R_1, R_2 are the principal radii of the coordinate lines curvature, τ_{ij} $(i, j = 1, 2)$ are the components of the surface stress tensor.

Let $\alpha_1 = x_1,\ \alpha_2 = x_2$ in the plane surface $x_3 = 0$. For the plane strain, we have $h_1 = h_2 = 1,\ 1/R_1 = 1/R_2 = 0$. As $\tau_{12} = 0,\ \tau_{22} = \tau_{22}(x_1)$, then according to Eq. (2), the boundary condition (1) in complex variables takes the form

$$\sigma_{33}(z) - i\sigma_{13}(z) = -ip(x_1) - it_s(x_1), \qquad z \in \Gamma, \tag{3}$$

where $p(x_1) = p_1(x_1) + ip_3(x_1)$; p_1, p_3 are the projections of the load vector **p** on the Cartesian coordinate axes x_1, x_3; $t_s = \partial\tau_{11}/\partial x_1$. Note that Eq. (3) can be directly derived considering an equilibrium of an element of a boundary surface under applied forces [5].

Generally, we assume that p(x) is the periodic function with the period a

$$p(x_1) = p(x_1 + a), \quad \int\limits_{x_1 - a/2}^{x_1 + a/2} p(t)dt = P, \quad P = P_1 + iP_3, \tag{4}$$

and satisfies the Hölder's condition on whole Γ. The following conditions are realized at infinity

$$\lim_{x_3 \to -\infty} (\sigma_{33}(z) - i\sigma_{13}(z)) = -iP/a, \quad \lim_{x_3 \to -\infty} \sigma_{11}(z) = \sigma_1, \quad \lim_{x_3 \to -\infty} \omega(z) = \omega^{\infty}, \tag{5}$$

where ω is the rotation angle of material particles; σ_{ij} are the stress components in the x_1, x_3 coordinate system.

The constitutive equations of linear elasticity for the surface [2, 7] and the bulk material in the case of the plane strain are reduced to the following

$$\tau_{11} = \gamma_0 + (\lambda_s + 2\mu_s - \gamma_0)\varepsilon_{11}^s, \quad \tau_{22} = \gamma_0 + (\lambda_s + \gamma_0)\varepsilon_{11}^s, \tag{6}$$

$$\begin{aligned} \sigma_{11} &= (\lambda + 2\mu)\varepsilon_{11} + \lambda\varepsilon_{33}, & \sigma_{33} &= (\lambda + 2\mu)\varepsilon_{33} + \lambda\varepsilon_{11}, \\ \sigma_{31} &= 2\mu\varepsilon_{31}, & \sigma_{22} &= \lambda(\varepsilon_{33} + \varepsilon_{11}), \end{aligned} \tag{7}$$

where γ_0 is the residual surface stress in an unstrained state; λ_s, μ_s are the moduli of surface elasticity similar to the Lamé constants λ, μ for 3D elasticity; ε_{ij} are the components of the strain in the bulk material; ε_{11}^s is the component of the surface strain.

3 Construction of Integral Equation

Proceeding from the volume Ω to the boundary Γ, we assume that the continuity condition of displacements is satisfied

$$\lim_{z \to x_1} u_j(z) = u_j^s(x_1),$$

where u_j^s is the displacement of points at the boundary Γ along the x_j-axis ($j = 1, 3$). This equality yields the continuity condition for the strain ε_{11}

$$\lim_{z \to x_1} \varepsilon_{11} = \varepsilon_{11}^s. \tag{8}$$

Relations (6) and (8) lead to the equation for finding the surface stress τ_{11}

$$\tau_{11}(x_1) = \gamma_0 + (\lambda_s + 2\mu_s - \gamma_0)\varepsilon_{11}(x_1), \tag{9}$$

Thus, the problem is reduced by defining a stress-strain state of the half-plane with the rectilinear boundary Γ on which the surface stress τ_{11} is acting. Equation (9) connects the unknown surface stress τ_{11} with the strain ε_{11} arising under external loading and conditions at infinity (5).

The expression for the strain ε_{11} can be found by solving the boundary problem (3), (5). The stress vector $\sigma_n = \sigma_{nn} + i\sigma_{nt}$ on the area with the normal $\mathbf{n}$ and the displacement vector $u = u_1 + iu_2$ of the point z are connected with the complex Goursat–Kolosov potentials by following formulas [4]

$$\sigma_n(z) = \Phi(z) + \overline{\Phi(z)} - \left(\Phi\,(\overline{z}) + \overline{\Phi(z)} - (z - \overline{z})\,\overline{\Phi'(z)}\right) e^{-2i\alpha}, \tag{10}$$

$$-\,2\mu\frac{du}{dz} = -\varkappa\Phi(z) + \overline{\Phi(z)} - \left(\Phi\,(\overline{z}) + \overline{\Phi(z)} - (z - \overline{z})\,\overline{\Phi'(z)}\right) e^{-2i\alpha}, \tag{11}$$

where α is the angle between the area and the axis x_1; $\varkappa = 3-4\nu$; ν is the Poisson's ratio. The derivative in Eq. (11) is taken along the area, i.e. in the direction of the vector $\mathbf{t}$ which is perpendicular to basis vector $\mathbf{n}$ so that n and t define the right-hand coordinate system.

The values of the function Φ at infinity follow from Eqs. (5), (10) and (11)

$$\begin{gathered}\lim_{x_3\to-\infty} \Phi(z) = \frac{\sigma_{11}^{\infty} + \sigma_{33}^{\infty}}{4} + \frac{2i\mu}{\varkappa+1}\omega^{\infty} = \frac{\sigma_1}{4} + \frac{P_3}{4a}\,, \\ \lim_{x_3\to-\infty} \Phi(\overline{z}) = \lim_{x_3\to-\infty} \Phi(z) - (\sigma_{33}^{\infty} - i\sigma_{13}^{\infty}) = \frac{\sigma_1}{4} + \frac{P_3}{4a} + \frac{iP}{a}\,.\end{gathered} \tag{12}$$

Let $z \to x_1 \in \Gamma$ and $\alpha = 0$ in Eq. (10). Then subjecting to the boundary conditions (3), we obtain Riemann–Hilbert's jump problem

$$\Phi^+(x_1) - \Phi^-(x_1) = it_s(x_1) + ip(x_1), \tag{13}$$

where $\Phi^{\pm}(x_1) = \lim\limits_{\mathrm{Im}\, z\to\pm0} \Phi(z)$. According to [9], the solution of the problem (13) can be written as

$$\Phi(z) - c^{\pm} = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{it_s(t)}{z-t}dt + \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{ip(t)}{z-t}dt = I_\tau(z) + I_p(z). \tag{14}$$

Here $c^{\pm} = \lim\limits_{x_3\to\pm\infty} \Phi(z) \mp iP/(2a)$, as $\lim\limits_{x_3\to\pm\infty} I_\tau(z) = 0$ and $\lim\limits_{x_3\to\pm\infty} I_p(z) = \pm iP/(2a)$.

Assuming $\alpha = \pi/2$ in Eq. (10) and then $\alpha = 0$ in Eq. (11), we obtain

$$\sigma_{11}(x_1) + i\sigma_{13}(x_1) = \Phi^-(x_1) + 2\overline{\Phi^-(x_1)} + \Phi^+(x_1), \tag{15}$$

$$-2\mu\frac{du}{dx_1} = -\varkappa\Phi^-(x_1) - \Phi^+(x_1). \tag{16}$$

Substituting Eq. (16) into (9) yields

$$\tau_{11} = \gamma_0 + M\mathrm{Re}\left(\varkappa\Phi^- + \Phi^+\right), \tag{17}$$

where $M = \dfrac{\lambda^s + 2\mu^s - \gamma_0}{2\mu}$.

Using the Sokhotski–Plemelj formulas, one can show that (17) is the integro - differential singular equation in surface stress τ_{11}. After differentiating Eq. (17) and using Eq. (14), we get the equation of the unknown function t_s

$$t_s(x_1) - M\mathrm{Re}\left(\varkappa I_\tau'^-(x_1) + I_\tau'^+(x_1)\right) = M\mathrm{Re}\left(\varkappa I_p'^-(x_1) + I_p'^+(x_1)\right). \tag{18}$$

In view of Eq. (14) and formulas Sokhotski-Plemelj, Eq. (18) yields

$$t_s(x_1) - \frac{M(\varkappa+1)}{2\pi}\int_{-\infty}^{+\infty}\frac{t_s(t)}{(t-x_1)^2}dt = \frac{M(\varkappa-1)}{2}p_3'(x_1) - \frac{M(\varkappa+1)}{2\pi}\int_{-\infty}^{+\infty}\frac{p_1(t)}{(t-x_1)^2}dt. \tag{19}$$

This hypersingular integral equation is obtained without using periodicity conditions of the function $p(x_1)$ and, therefore, it is valid for an arbitrary loading. In case of non-periodic loadings, the function p should vanish at infinity and satisfy to conditions of integral existence in the right hand side of Eq. (19) in sense of Hadamard's finite part [8].

It should be noticed that the homogeneous equation corresponding to Eq. (19) has only zero solution. Otherwise, under the absence of external loadings, there would be a surface stress τ_{11} differing from a constant that for an infinite plane surface is unreal. Therefore, if a derivative of function t_s satisfies to Hölder's condition, then Eq. (19) always has the unique solution for any continuous right hand side of Eq. (19) [8].

4 Solution of Equation (19) in the Case of Periodic Loading

Find the solution of the integral Eq. (19) in the case of the action of a self-balanced periodic loading at the boundary Γ, i.e. assume that $P = 0$ in Eq. (4). Consider a special case when tangential load p_1 is described by an odd function, and normal load p_3 – by an even one. Then function p can be expanded into the following Fourier series

$$p(x) = p_1(x) + ip_3(x) = \sum_{k=1}^{\infty} C_k \sin b_k x + i \sum_{k=1}^{\infty} D_k \cos b_k x, \qquad (20)$$

where

$$C_k = \frac{2}{a} \int_{-a/2}^{a/2} p_1(x) \sin b_k x dx, \quad D_k = \frac{2}{a} \int_{-a/2}^{a/2} p_3(x) \cos b_k x dx, \quad b_k = 2\pi k/a.$$

Hereinafter, we will denote $x \equiv x_1$ instead of x_1.

We also calculate the function t_s in the form of Fourier series

$$t_s(x) = \sum_{k=1}^{\infty} A_k \sin b_k x + B_k \cos b_k x. \qquad (21)$$

It is possible to find unknown factors A_k, B_k from Eq. (19) by substituting the expressions (20) and (21) into it and computing corresponding integrals. However, there exists a more convenient method to find these factors. Using Eqs. (14), (20) and (21), we derive the following expression for complex potential Φ

$$\Phi(z) = \frac{\sigma_{11}^{\infty}}{4} + \frac{1}{2} \sum_{k=1}^{\infty} \begin{cases} (C_k - D_k + A_k + iB_k)e^{ib_k z}, & \operatorname{Im} z > 0, \\ (C_k + D_k + A_k - iB_k)e^{-ib_k z}, & \operatorname{Im} z < 0. \end{cases} \qquad (22)$$

After substituting Eq. (22) into Eq. (18) and using definitions (14), we equate the coefficients at the same harmonics that yields

$$A_k = -\frac{\pi k \left(C_k(\varkappa + 1) + D_k(\varkappa - 1)\right)}{a/M + \pi k(\varkappa + 1)}, \quad B_k = 0, \quad k = 1, 2, \ldots \qquad (23)$$

Thus, we have obtained analytical expressions for all coefficients in the Fourier series (21) of function t_s. In other words, we have got the exact solution of the integral Eq. (19) in the form of Fourier series.

Integrating Eq. (21), we derive the expression for the surface stress

$$\tau_{11}(x) = -\sum_{k=1}^{\infty} \frac{A_k}{b_k} \cos b_k x + \tau_0. \qquad (24)$$

The constant τ_0 can be found from Eq. (17). For this purpose, substitute Eqs. (22) and (24) into Eq. (17). Then, assuming $C_k = D_k = 0$ $(k = 1, 2, \ldots)$ in the derived equation, that corresponds to a free boundary of the half-plane, we obtain

$$\tau_0 = \gamma_0 + \frac{M(1+\varkappa)}{4}\sigma_1. \tag{25}$$

The quantity τ_0 is the surface stress corresponding to a homogeneous stress-strain state of bulk material with a plane boundary. As one can see from Eq. (25), $\tau_0 = \gamma_0$ for an unloaded body. So if $\sigma_1 = 0$, and the boundary is free from the external loading, there are no deformations in the bulk material and in the surface as well. In the general case, surface stress τ_0 depends on both γ_0 and σ_1.

Substituting Eq. (22) into Eq. (15), we obtain expressions for longitudinal σ_{11} and tangential σ_{13} stresses at Γ

$$\begin{aligned} \sigma_{11}(x)|_{x_3=0} &= \sum_{k=1}^{\infty}\left(2C_k + D_k + 2A_k\right)\cos b_k x + \sigma_1, \\ \sigma_{13}(x)|_{x_3=0} &= -\sum_{k=1}^{\infty}\left(C_k + A_k\right)\sin b_k x. \end{aligned} \tag{26}$$

5 Example

Let the external loads at the boundary of the half-plane be defined by one of the following functions

$$p_1(x) = q_1 \mathrm{Im}\, f / \max|\mathrm{Im}\, f|, \quad p_3(x) = q_3 \mathrm{Re}\, f / \max|\mathrm{Re}\, f|, \tag{27}$$

where $f(x) = -\,\mathrm{sh}^{-2}\,(y + i\pi x/a)$; q_1, q_3 are the dimension factors equal to maximum of absolute values of corresponding loads; the parameter y defines a form of corresponding curves. The plots of functions (27) for $y = 0.5$ are represented in Fig. 1 by continuous lines. As it follows from Eq. (27), $p_1(x) \to q_1 \sin(2\pi x/a)$, $p_3(x) \to -q_3 \cos(2\pi x/a)$, when $y \to \infty$.

Approximating each of functions (27) by a piece of the corresponding Fourier series (20) with prescribed accuracy ε, one can obtain the numerical solution of the problem with the same accuracy. As a criterion of accuracy, we accept an integral criterion. According to it, a ratio of the difference between the integral of function p_j and of its approximation over an interval of positive changing to the first one does not exceed a given value ε.

The results of calculations show that the number of members of the corresponding series required for an achievement of the prescribed accuracy depends on the value of parameter y. This number increases if y decreases. In particular, when $y = 0.5$, five members of the series are enough to approximate the function $p_1(x_1)$ with the accuracy $\varepsilon = 0.01$.

For comparison, we also consider the action of tangential and normal loads defined by the first member of Fourier series (20) and represent them by dashed lines in Fig. 1. They also can be defined by the corresponding functions (27) if $y \to \infty$

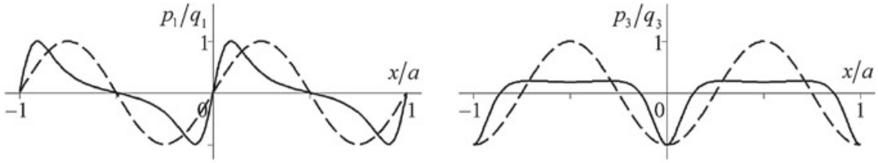

Fig. 1 Two types of tangential p_1 and normal p_3 external loads for $y = 0.5$ (*continuous lines*) and $y = \infty$ (*dotted*) in (27)

$$p_1(x) = q_1 \sin b_1 x, \quad p_3(x) = -q_3 \cos b_1 x. \tag{28}$$

Using formulas (20), (23) and (26), we calculated stresses at the boundary for various values of geometrical parameters a and y with and without surface stress τ_{11}. Loads are defined by functions (27) when $y = 0.5$ and functions (28). Besides, for simplification of an analysis, it is assumed that $\sigma_1 = 0$. The Poisson's ratio $\nu = 0.3$.

The plots of dependencies of the maximum absolute values of longitudinal and tangential stresses on the period of loadings a are displayed in Fig. 2. Continuous lines correspond to loadings (27), dotted - to (28). These dependencies illustrate the so-called size effect noticed at the nanoscale in many works (see, for example, [1, 3, 6, 11]) if the surface stress is taken into account.

From Fig. 2 one can conclude that the most significant influence of the period of loading a on stresses is in the limits of changing a approximately from 10 M to 300 M. For aluminum $M = 0.113$ nm [2], and this period is in the interval from 1 to 34 nm. If $a > 1000\,M$, the size effect almost disappears and the stress-strain state of a body does not depend on the surface stress.

Note that the size effect becomes more apparent for the tangential loads (curves 1) than for the normal (curves 2). Besides, the maximum values of stress σ_{11} are less for sinusoidal loadings (28) than for loadings (27). For the maximum values of stress σ_{13}, the behavior is opposite. The plots of stresses at the boundary of the half-plane are

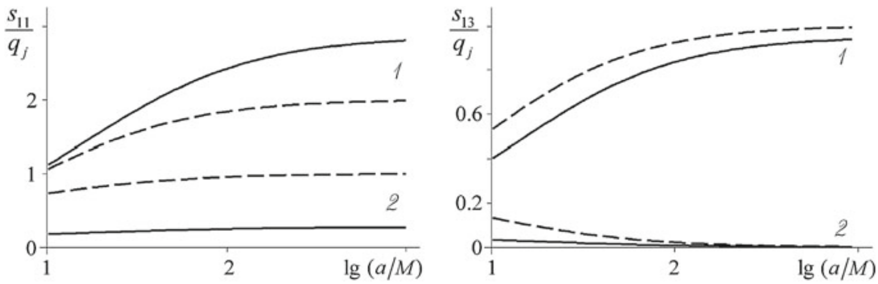

Fig. 2 The maximum of the absolute value of the longitudinal stress $s_{11} = \max|\sigma_{11}|$ and tangential stress $s_{13} = \max \sigma_{13}$ versus the period a for tangential loadings (*curves 1*) and normal loadings (*curves 2*)

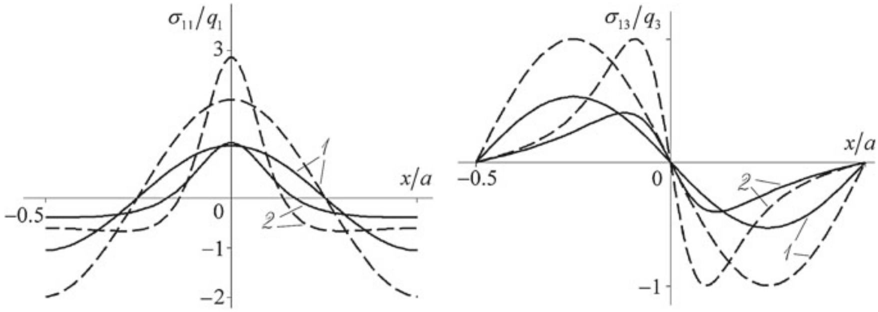

Fig. 3 The distribution of longitudinal σ_{11} and tangential σ_{13} stresses on the half-plane boundary in the range of one period for tangential loadings and $a = 10\,M$

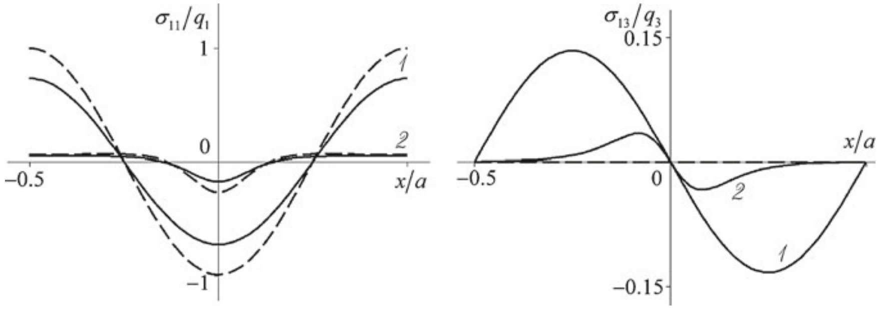

Fig. 4 The distribution of longitudinal σ_{11} and tangential σ_{13} stresses on the half-plane boundary in the range of one period for normal loadings and $a = 10\,M$

represented in Figs. 3 and 4 by continuous and dashed lines calculated with and without the surface stress respectively. Curves 1 corresponds to the action of loads (28), curves 2—loads (27) if $y = 0.5$. The plots are constructed for $a = 10\,M$. For such value of a, the difference between the solution with the surface stress and the traditional solution is clearly expressed.

It is apparent from the dependencies given in Figs. 3 and 4 that the existence of a surface stress reduces the concentration of longitudinal and tangential stresses. As a result, changing of these stresses becomes more smooth than it predicts the solution in traditional statement. It is remarkable that, owing to the surface stress, normal loadings cause tangential stresses at the boundary (Fig. 4). This fact follows directly from boundary conditions (3) which mean that if the surface stress is not constant, then the tangential stress will always be at the half-plane boundary independently of the type of loading.

It is interesting to estimate an influence of the surface stress on the relative changes of extremal values of stresses at the boundary for loadings defined by function (27) with $y = 0.5$ and function (28). This influence can be seen from Table 1 in which these extremal values corresponding to graphs in Figs. 3 and 4 are given.

Table 1 Extreme values of stresses at the boundary versus type of loading for $a = 10$, $M = 1.13$ nm

Type of loading		Tangent loading p_1/q_1		Normal loading p_3/q_3	
Type of function		Func. Eq. (27)	Func. Eq. (28)	Func. Eq. (27)	Func. Eq. (28)
max σ_{11}	$\tau_{11} = 0$	2.855	2	0.064	1
	$\tau_{11} \neq 0$	1.120	1.064	0,047	0.733
min σ_{11}	$\tau_{11} = 0$	−0.668	−2	−0.272	−1
	$\tau_{11} \neq 0$	−0.394	−1.064	−0.177	−0.733
max σ_{13}	$\tau_{11} = 0$	0.882	1	0	0
	$\tau_{11} \neq 0$	0.401	0.532	0.034	0.134

6 Conclusion

The stress state of an elastic half-plane under the action of periodic surface forces at the nanoscale is investigated. Based on the Gurtin–Murdoch model of surface elasticity, complex potentials of Goursat–Kolosov, the Muskhelishvili representations and boundary properties of analytical functions, the solution of the boundary value problem in the general case of arbitrary loading at the boundary is reduced to the hypersingular integral equation. The exact solution of this equation in the form of Fourier series is obtained in the case of periodic loading. The numerical results for aluminum show that the highest influence of the surface stress on the stress state of the boundary takes place when the loading period does not exceed approximately 40 nm. As follows from the solution (23), this influence depends on elastic constants of the surface and bulk material, by which the parameter M is expressed.

It is important to note one feature of the considered boundary problem. The surface stress arises in a planar surface as a reaction on the changing the external load along the surface. So far, the existence of the surface stress has been considered in a curved boundary surface that is free from external loading (see, for example, [2, 3, 5–7, 11]). In this sense, there is a steady opinion that the surface stress appears only on a curvilinear surface, and the size effect is expressed in a dependence of physical properties and stress-strain state of a body on the change of the surface curvature.

In this work, the surface of the body has a zero curvature and a geometrical linear dimension to which the size effect is related is the period of the load. Another feature of the solution obtained is that the surface stress appears from the action of normal loads and this leads to arising tangential stresses. As in the case with size effect, these stresses become negligible when the period a is 100 nm. or more.

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