PAPER REF: 4073

HARMONIC OSCILLATIONS OF NANOSIZE PIEZOELECTRIC BODIES WITH SURFACE EFFECTS

Andrey V. Nasedkin [1(*)], Victor A. Eremeyev [2]
[1]Department of Mathematic Modeling, Southern Federal University, Rostov on Don, Russia
[2]Otto-von-Guericke-University at Magdeburg, Magdeburg, Germany
[(*)]*Email:* nasedkin@math.sfedu.ru

ABSTRACT

The paper considers the harmonic and eigenvalue problems for piezoelectric nanodimensional bodies with account for surface stresses and surface electric charges. For harmonic problem the new mathematical model is suggested, which generalize the model of the piezoelectric medium with damping properties, boundary conditions of contact type and surface effects. The classical and generalized or weak statements for harmonic and eigenvalue problems are obtained in the extended and reduced forms. The spectral properties of the eigenvalue problems with account for surface effects are determined. A variational principle is constructed which has the properties of minimality, similar to the well-known variational principle for problems with pure elastic and piezoelectric media. The discreteness of the spectrum and completeness of the eigenvectors are proved. As a consequence of variational principles, the properties of an increase or a decrease in the natural frequencies, when the mechanical, electric and "surface" boundary conditions and the moduli of piezoelectric solid change, are established. The finite element approaches are described for determination of the natural frequencies, the resonance and antiresonance frequencies and harmonic behavior of nanosize piezoelectric bodies with account for surface effects.

Keywords: piezoelectricity, nanomechanics, surface effect, surface stress, harmonic oscillations, eigenvalue, resonance frequencies, finite element method

INTRODUCTION

As it is known, nanomaterials has abnormal mechanical properties which differ considerably from conventional macromaterials. One of the factors that are responsible of the behavior of nanomaterials can be surface effects. As recent investigations (see, for example, Duan, 2005, Duan, 2006, Jing 2006) show, that for the bodies of submicro-and nanosize the surface stresses play an important role and influence the deformation of the bodies in general. Similar to the elastic bodies, when analyzing the piezoelectric nanosize media one can introduce surface stresses and distributed electric charges into the model by adding to the surface the corresponding elastic membranes and dielectric films. This approach is used in the present work for investigations of the vibrations of piezoelectric nanosize bodies.

CLASSICAL FORMULATION OF HARMONIC PROBLEM FOR PIEZOELECTRIC BODY WITH SURFACE EFFECTS

Let Ω be a bounded in R^3 region, occupied by the piezoelectric body; $\Gamma = \partial\Omega$ is the boundary of the region, $\mathbf{n}$ is the vector of the external unit normal to Γ. Confining ourselves to the consideration of the stationary oscillations regimes with the circular frequency ω, we will use only amplitude values of all physical-mechanical variable hereinafter without special reference. Let us consider the vector of mechanical displacements $\mathbf{u} = \mathbf{u}(\mathbf{x})$ and the electric potential $\varphi = \varphi(\mathbf{x})$ as the main variables for the piezoelectric medium. Using these functions, we can define the second-order strain tensor $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}(\mathbf{u})$ and the electric field vector $\mathbf{E} = \mathbf{E}(\varphi)$

$$\boldsymbol{\varepsilon} = (\nabla\mathbf{u} + \nabla\mathbf{u}^T)/2, \qquad \mathbf{E} = -\nabla\varphi, \tag{1}$$

where ∇ is the nabla-operator, and in R^3 in the Cartesian coordinate system $\nabla = \{\partial/\partial x_1, \partial/\partial x_2, \partial/\partial x_3\}$; $(...)^T$ is the transpose operation.

In linear approximation similarly to (Nasedkin, 2000) we adopt the following constitutive equations for piezoelectric medium

$$\boldsymbol{\sigma} = (1 + j\omega\beta_d)\mathbf{c}\cdot\cdot\boldsymbol{\varepsilon} - \mathbf{e}^T\cdot\mathbf{E}, \tag{2}$$

$$\mathbf{D} = \mathbf{e}\cdot\cdot\boldsymbol{\varepsilon} + (1 + j\omega\varsigma_d)^{-1}\boldsymbol{\kappa}\cdot\mathbf{E}, \tag{3}$$

where $\boldsymbol{\sigma}$ is the second-order stress tensor; $\mathbf{D}$ is the electric displacement vector; $\mathbf{c} = \mathbf{c}^E$ is the forth-order tensor of elastic modules, measured at constant electric field; $\mathbf{e}$ is the third-order tensor of piezomoduli; $\boldsymbol{\kappa} = \boldsymbol{\kappa}^S$ is the second-order tensor of dielectric permittivities, measured at constant strain (usually, tensor of dielectric permittivities denote as $\boldsymbol{\varepsilon}^S$, i.e. here $\boldsymbol{\kappa}^S = \boldsymbol{\varepsilon}^S$); β_d and ς_d are the damping coefficients. (Here the conventional for the piezoelectricity theory superscripts at $\mathbf{c}^E$ and $\boldsymbol{\kappa}^S$ ($\boldsymbol{\kappa}^S = \boldsymbol{\varepsilon}^S$) are omitted for the compactness of further notations.)

The equation of motion and equation of quasielectrostatics for the harmonic problem can be written in the form

$$\nabla\cdot\boldsymbol{\sigma} + \rho\mathbf{f} = \rho(-\omega^2 + j\omega\alpha_d)\mathbf{u}, \tag{4}$$

$$\nabla\cdot\mathbf{D} = q_\Omega, \tag{5}$$

where ρ is the mass density of the material; $\mathbf{f}$ is the vector of mass forces; α_d is the additional damping coefficient; q_Ω is the density of free electric charges (usually, $q_\Omega = 0$).

In models (1)-(5) for the piezoelectric material, we use a generalized Rayleigh method of damping evaluation (Belokon, 2002, Nasedkin, 2010), which is admissible for many practical applications. When $\varsigma_d = 0$ in Eq. (3), we have the usual model for taking into account of mechanical damping in piezoelectric media which is adopted in several well-known finite element packages. It is true that, by virtue of the coupled state of the mechanical and electric fields, the damping effects will also extend into the electric fields when $\varsigma_d = 0$. More complicated model (2), (3) extends the Kelvin's model to the case of piezoelectric media. It has been shown that the model (2), (3) with $\beta_d = \varsigma_d$ satisfies the conditions of the energy dissipation and has the possibility of splitting the finite element system into independent equations for the separate modes (Belokon, 2002).

The density $\rho(\mathbf{x})$ is assumed to be piecewise-continuous and $\exists\ \rho_0 > 0$: $\rho(\mathbf{x}) \ge \rho_0$. The material modules of the medium in (2), (3) are piecewise-continuous together with their first derivatives by $\mathbf{x}$ with usual symmetry conditions ($c_{ijkl} = c_{jikl} = c_{klij}$, $e_{ikl} = e_{ilk}$, $\kappa_{kl} = \kappa_{lk}$), and for the positive definite volume density of internal energy $W(\boldsymbol{\varepsilon},\mathbf{E})$ the following inequality should satisfy $\forall\ \boldsymbol{\varepsilon}=\boldsymbol{\varepsilon}^T$, $\mathbf{E}$

$$\exists\ c_W>0: \qquad W(\boldsymbol{\varepsilon},\mathbf{E})=\frac{1}{2}(\boldsymbol{\varepsilon}\cdot\cdot\mathbf{c}\cdot\cdot\boldsymbol{\varepsilon}+\mathbf{E}^T\cdot\boldsymbol{\kappa}\cdot\mathbf{E})\ge c_W(\boldsymbol{\varepsilon}\cdot\cdot\boldsymbol{\varepsilon}+\mathbf{E}^T\cdot\mathbf{E})\,. \tag{6}$$

The system of differential equations (4), (5) should be completed by the suitable boundary conditions. These boundary conditions can be divided in two types, mechanical and electric.

To formulate the mechanical boundary conditions we assume that the boundary Γ is divided in two subsets Γ_σ and Γ_u ($\Gamma=\Gamma_\sigma\cup\Gamma_u$).

We will assume that at the part of the boundary Γ_σ there are the surface stresses $\boldsymbol{\tau}^s$ and the vector of mechanical stress $\mathbf{p}_\Gamma$

$$\mathbf{n}\cdot\boldsymbol{\sigma}=\nabla^s\cdot\boldsymbol{\tau}^s+\mathbf{p}_\Gamma\,, \qquad \mathbf{x}\in\Gamma_\sigma\,, \tag{7}$$

where ∇^s is the surface gradient operator, associated with nabla-operator by the formula $\nabla^s=\nabla-\mathbf{n}\,\partial/\partial r$; r is the coordinate, measured by the normal to Γ_σ; $\boldsymbol{\tau}^s$ is the second-order tensor of surface stresses.

As for purely elastic body, when taking into account the surface stresses and the Kelvin's damping model we adopt that the surface stresses $\boldsymbol{\tau}^s$ are related to the surface strains $\boldsymbol{\varepsilon}^s$ by the formula

$$\boldsymbol{\tau}^s=(1+j\omega\beta_d^s)\mathbf{c}^s\cdot\cdot\boldsymbol{\varepsilon}^s\ , \qquad \boldsymbol{\varepsilon}^s=(\nabla^s\mathbf{u}\cdot\mathbf{A}+\mathbf{A}\cdot(\nabla\mathbf{u}^s)^T)/2\,, \tag{8}$$

where β_d^s is the new damping coefficient; $\mathbf{c}^s$ is the forth-order tensor of surface elastic modules; $\mathbf{A}=\mathbf{I}-\mathbf{n}\otimes\mathbf{n}$, $\mathbf{I}$ is the unit tensor in R^3.

The properties of the tensor of surface elastic modules $\mathbf{c}^s$ are analogous to the corresponding properties of the tensor $\mathbf{c}$, i.e. $c^s_{ijkl}=c^s_{jikl}=c^s_{klij}$,

$$\exists\ c_U>0: \qquad \forall\ \boldsymbol{\varepsilon}^s=\boldsymbol{\varepsilon}^{sT} \qquad U(\boldsymbol{\varepsilon}^s)=\frac{1}{2}\boldsymbol{\varepsilon}^s\cdot\cdot\mathbf{c}^s\cdot\cdot\boldsymbol{\varepsilon}^s\ge c_U\boldsymbol{\varepsilon}^s\cdot\cdot\boldsymbol{\varepsilon}^s\,, \tag{9}$$

that follow from the condition of the positive definiteness of the surface energy density $U(\boldsymbol{\varepsilon}^s)$.

Suppose that $\Gamma_u=\cup_i\Gamma_{ui}$; $i=0,1,2,...,L$; $\Gamma_{u0}\ne\wedge$, Γ_{ui} do not border one another; while among Γ_{ui} there are $L+1-l$ surfaces with given functions of displacement $\mathbf{u}=\mathbf{u}_\Gamma$ ($i\in J_r=\{0,l+1,l+2,...,L\}$) and l plane regions ($i\in J_p=\{1,2,...,l\}$), in friction-free contact with rigid massive punches (stamps). We will connect with region Γ_{ui}, $i\in J_p$ the local coordinate system $O_\xi^{(i)}\xi_1^{(i)}\xi_2^{(i)}\xi_3^{(i)}$ so that the axis $\xi_3^{(i)}$ coincides in direction with the direction of external normal $\mathbf{n}$ at the point $O_\xi^{(i)}$; and the axes $\xi_1^{(i)}$ and $\xi_2^{(i)}$ will be the main axes of inertia for the punch with number i (Fig. 1). Then, we can assume the following boundary conditions for Γ_{ui}

$$\mathbf{n}\cdot\mathbf{u}=\sum_{k=0}^{2}\alpha_{ik}^{u}\xi_{k}^{(i)}\,,\qquad (\xi_{0}^{(i)}=1),\qquad \mathbf{x}\in\Gamma_{ui}\,,\qquad i\in J_{p}\,, \tag{10}$$

$$\int_{\Gamma_{ui}}\xi_{p}^{(i)}\mathbf{n}\cdot\boldsymbol{\sigma}\cdot\mathbf{n}\,d\Gamma=(\omega^{2}-j\omega\alpha_{d}^{p})\alpha_{ip}^{u}M_{p}^{(i)}+P_{ip}\,,\qquad p=0,1,2\,,\qquad i\in J_{p}\,, \tag{11}$$

$$\mathbf{n}\cdot\boldsymbol{\sigma}-(\mathbf{n}\cdot\boldsymbol{\sigma}\cdot\mathbf{n})\mathbf{n}=\nabla^{s}\cdot\boldsymbol{\tau}^{s}\,,\qquad \mathbf{x}\in\Gamma_{ui}\,,\qquad i\in J_{p}\,, \tag{12}$$

$$\mathbf{u}=\mathbf{u}_{\Gamma i}\,,\qquad \mathbf{x}\in\Gamma_{ui}\,,\qquad \Gamma_{u0}\neq\wedge\,,\qquad i\in J_{r}\,, \tag{13}$$

where in (10), (11) the summation by repeating index i and p is missing; α_{i0}^{u} is the normal displacement of the punch with number i; $\alpha_{i1}^{u}=-\theta_{2}^{(i)}$, $\alpha_{i2}^{u}=\theta_{1}^{(i)}$ are the punch rotation angles about axes $\xi_{2}^{(i)}$ and $\xi_{1}^{(i)}$, respectively; $M_{0}^{(i)}$ is the mass of punch; $M_{1}^{(i)}=J_{\xi_{2}^{(i)}\xi_{2}^{(i)}}$, $M_{2}^{(i)}=J_{\xi_{1}^{(i)}\xi_{1}^{(i)}}$ are the inertia moments of punch; P_{ip} are the force (with $p=0$) and the moments (with $p=1,2$), acting on the punch with number k; α_{d}^{p} is the damping coefficient for massive punches motion; $\mathbf{u}_{\Gamma i}=\mathbf{u}_{\Gamma i}(\mathbf{x})$ are the components of determined functions of displacements on Γ_{ui}, $i\in J_{r}$.

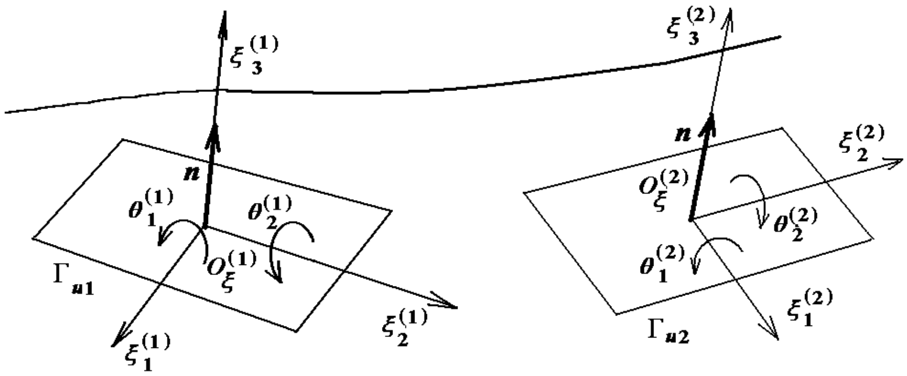

Fig. 1. Contact type boundaries with plane punches.

Note that here in friction-free contact between nanodimensional body and rigid punches the tangential stresses are not equal to zero, but are balanced by (12) to the effect of surface stresses, as in (7).

To set the electric boundary conditions we assume that the surface Γ is also subdivided in two subsets: Γ_D and Γ_φ ($\Gamma=\Gamma_D\cup\Gamma_\varphi$).

The regions Γ_D does not contain electrodes and hold the following conditions

$$\mathbf{n}\cdot\mathbf{D}=\nabla^{s}\cdot\mathbf{d}^{s}-q_{\Gamma}\,,\quad \mathbf{x}\in\Gamma_{D}\,, \tag{14}$$

where $\mathbf{d}^{s}=(1+j\omega\zeta_{d}^{s})^{-1}\mathbf{A}\cdot\boldsymbol{\kappa}^{s}\cdot\mathbf{A}\cdot\mathbf{E}^{s}$; ζ_{d}^{s} is the additional new damping coefficient; $\mathbf{E}^{s}=-\nabla^{s}\varphi$; $\boldsymbol{\kappa}^{s}$ is the second-order dielectric permittivity tensor that is symmetrical positive definite relatively to the vectors $\mathbf{E}^{s}$; q_{Γ} is the known surface density of electric charge, and usually, $q_{\Gamma}=0$.

As it can be seen, here analogously to the boundary condition (7) at the free of electrodes boundaries Γ_D we take into account the influence of the surface films with the vectors of surface electric displacement $\mathbf{d}^s$ and with the vectors of surface electric field $\mathbf{E}^s$.

The subset Γ_φ is the union of $M+1$ regions $\Gamma_{\varphi i}$ ($i \in J_Q \cup J_V$), $J_Q = \{1, 2, ..., m\}$, $J_V = \{0, m+1, m+2, ..., M\}$), that does not border on each other and are covered with infinitely thin electrodes. At these regions we set the following boundary conditions

$$\varphi = \Phi_i, \qquad \mathbf{x} \in \Gamma_{\varphi i}, \qquad i \in J_Q, \tag{15}$$

$$\int_{\Gamma_{\varphi i}} \mathbf{n} \cdot \mathbf{D}\, d\Gamma = -Q_i, \quad I_i = \pm j\omega Q_i, \quad i \in J_Q, \tag{16}$$

$$\varphi = V_i, \qquad \mathbf{x} \in \Gamma_{\varphi i}, \qquad \Gamma_{\varphi 0} \neq \wedge, \qquad i \in J_V, \tag{17}$$

where the variables Φ_i, V_i do not depend on $\mathbf{x}$; Q_i is the overall electric charge on electrode $\Gamma_{\varphi i}$, and the sign "$\pm$" in (16) is chosen in accordance with the accepted direction of the current I_i in the electric circuit.

According to (15), (16) over the parts $\Gamma_{\varphi i}$ the electric potential Φ_i is the same but unknown a priori, and the additional condition to define this is the integral condition (16). Such electrodes $\Gamma_{\varphi i}$ with $i \in J_Q$ can be named as electrodes with independent currents or charges sources. For $I_i = 0$ these electrodes are called also as open-circuited electrodes. The second set of electrodes $\Gamma_{\varphi i}$ with $i \in J_V$ can be named as electrodes with independent voltage sources. For $V_i = 0$ these electrodes are called also as short-circuited electrodes.

Let us note that in (15) and (17) Φ_i and V_i are free of space coordinate $\mathbf{x}$, and so, the boundaries $\Gamma_{\varphi i}$ are equipotential surfaces. Integral condition (16) is an analogue to the contact condition for rigid punches. But the distinctive feature of the piezoelectric devices is that boundary conditions (15) – (17) are necessary for them, since they determine the outer electric influence between Φ_i, V_i, Q_i or I_i.

Note that here the electric surface effects are taken into account by introducing the member with the vector of surface electric displacements $\mathbf{d}^s$ into relation (14). On the regions $\Gamma_{\varphi i}$ surface electric displacements are equal to zero, because on $\Gamma_{\varphi i}$ electric potential is not depend from coordinates $\mathbf{x}$, and therefore, $\mathbf{E}^s = 0$, $\mathbf{d}^s = 0$.

Problem (1) – (17) is the classical formulation of the harmonic problem for piezoelectric body with the generalized Rayleigh damping and with account for surface effects.

Observe that the boundary conditions (10) – (12) for plane rigid punches usually are absent, i.e. $J_p = \wedge$, $l = 0$. We introduce these unconventional cases of contact conditions with rigid punches to demonstrate an analogy between these mechanical boundary conditions and electric boundary conditions for electrode surfaces.

As an example, a variant of mechanical boundary conditions (10) – (13) for $L = 4$, $l = 2$ and a variant of electric boundary conditions (15) – (17) for $M = 3$, $m = 1$ are shown on Fig. 2, (left and right, respectively).

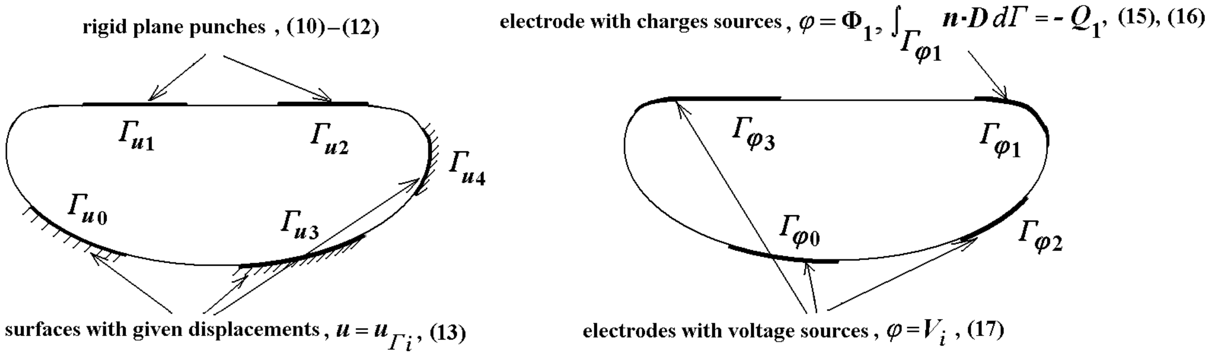

Fig. 2. Example of mechanical and electric boundary conditions.

GENERALIZED OR WEAK PROBLEM STATEMENTS

We transfer from the classical formulation (1) – (17) of the harmonic problem for piezoelectric bodies with the generalized Rayleigh damping and with account for surface effects to their generalized or weak settings.

Previously we introduce the complex valued space of the functions φ and the vector functions $\mathbf{u}$, defined on Ω. We denote by H_ρ^0 the space of vector functions $\mathbf{u} \in L_2$ with scalar product $(\mathbf{v},\mathbf{u})_{H_\rho^0} = \int_\Omega \rho \overline{\mathbf{v}}^T \cdot \mathbf{u}\, d\Omega$, where $\overline{(...)}$ is the complex conjugation operation.

On the set of vector functions $\mathbf{u} \in C^1$ which satisfy homogeneous boundary condition (13) $\mathbf{u} = 0$ on Γ_{ui}, $i \in J_r$, and (10) for arbitrary α_{ik}^u for Γ_{ui}, $i \in J_p$, we introduce the scalar product $(\mathbf{v},\mathbf{u})_{H_u^1} = \int_\Omega (\nabla \overline{\mathbf{v}})^T \cdot\cdot \nabla \mathbf{u}\, d\Omega + \int_{\Gamma_\tau} (\mathbf{A} \cdot \nabla^s \overline{\mathbf{v}})^T \cdot\cdot (\nabla^s \mathbf{u} \cdot \mathbf{A})\, d\Gamma$; $\Gamma_\tau = \Gamma_\sigma \cup (\cup_{i \in J_p} \Gamma_{ui})$. The closure of this set of vector functions $\mathbf{u}$ in the norm generated by the indicated scalar product will be denoted by H_u^1.

For functions $\varphi \in C^1$ which satisfy homogeneous boundary condition (17) $\varphi = 0$ on $\Gamma_{\varphi i}$, $i \in J_V$, and (15) for arbitrary Φ_i on $\Gamma_{\varphi i}$, $i \in J_Q$ we introduce the scalar product $(\chi,\varphi)_{H_\varphi^1} = \int_\Omega (\nabla \overline{\chi})^T \cdot \nabla \varphi\, d\Omega + \int_{\Gamma_D} (\nabla^s \overline{\chi})^T \cdot \nabla^s \varphi\, d\Gamma$. The closure of this set of functions φ in the norm generated by the indicated scalar product will be denoted by H_φ^1.

In order to formulate the generalized or weak solution of harmonic problem we scalar multiply equation (4) by arbitrary vector function $\overline{\mathbf{v}} \in H_u^1$, and we multiply equation (5) by some function $\overline{\chi} \in H_\varphi^1$. By integrating the obtained equations on Ω, and by using the standard technique of the integration by parts with Eqs. (1) – (3), (7), (8), (10) – (17), we obtain the following integral relations

$$\begin{aligned} &(-\omega^2 + j\omega\alpha_d)\rho(\mathbf{v},\mathbf{u}) + (-\omega^2 + j\omega\alpha_d^p)\rho_P(\mathbf{v},\mathbf{u}) + \\ &+ (1 + j\omega\beta_d)c_\Omega(\mathbf{v},\mathbf{u}) + (1 + j\omega\beta_d^s)c_\Gamma(\mathbf{v},\mathbf{u}) + e(\varphi,\mathbf{v}) = \widetilde{L}_u(\mathbf{v}), \end{aligned} \tag{18}$$

$$-e(\chi,\mathbf{u}) + (1 + j\omega\varsigma_d)^{-1}\kappa_\Omega(\chi,\varphi) + (1 + j\omega\varsigma_d^s)^{-1}\kappa_\Gamma(\chi,\varphi) = \widetilde{L}_\varphi(\chi), \tag{19}$$

where

$$\rho(\mathbf{v},\mathbf{u}) = (\mathbf{v},\mathbf{u})_{H^0_\rho}, \qquad \rho_P(\mathbf{v},\mathbf{u}) = \sum_{i=1}^{l}\sum_{k=0}^{2} \overline{\alpha}^v_{ik}\alpha^u_{ik} M^{(i)}_k, \tag{20}$$

$$c_\Omega(\mathbf{v},\mathbf{u}) = \int_\Omega \boldsymbol{\varepsilon}(\overline{\mathbf{v}})\cdot\cdot\,\mathbf{c}\cdot\cdot\,\boldsymbol{\varepsilon}(\mathbf{u})\,d\Omega, \qquad c_\Gamma(\mathbf{v},\mathbf{u}) = \int_{\Gamma_\tau} \boldsymbol{\varepsilon}^s(\overline{\mathbf{v}})\cdot\cdot\,\mathbf{c}^s\cdot\cdot\,\boldsymbol{\varepsilon}^s(\mathbf{u})\,d\Gamma, \tag{21}$$

$$e(\varphi,\mathbf{v}) = -\int_\Omega \mathbf{E}(\varphi)\cdot\mathbf{e}\cdot\cdot\,\boldsymbol{\varepsilon}(\overline{\mathbf{v}})\,d\Omega, \tag{22}$$

$$\kappa_\Omega(\chi,\varphi) = \int_\Omega \mathbf{E}(\overline{\chi})\cdot\boldsymbol{\kappa}\cdot\mathbf{E}(\varphi)\,d\Omega, \qquad \kappa_\Gamma(\chi,\varphi) = \int_{\Gamma_D} \mathbf{E}^s(\overline{\chi})\cdot\boldsymbol{\kappa}^s\cdot\mathbf{E}^s(\varphi)\,d\Gamma, \tag{23}$$

Further, we present the solution $\{\mathbf{u},\varphi\}$ of the harmonic problem in the form

$$\mathbf{u} = \mathbf{u}_0 + \mathbf{u}_b, \qquad \varphi = \varphi_0 + \varphi_b, \tag{24}$$

where $\mathbf{u}_0$, φ_0 satisfy homogeneous boundary mechanical and electric conditions and $\mathbf{u}_b$, φ_b satisfy the inhomogeneous boundary conditions, i.e.

$$\mathbf{n}\cdot\mathbf{u}_0 = \sum_{k=0}^{2}\alpha^{u0}_{ik}\xi^{(i)}_k, \quad \mathbf{n}\cdot\mathbf{u}_b = \sum_{k=0}^{2}\alpha^{ub}_{ik}\xi^{(i)}_k, \quad \alpha^{u0}_{ik} + \alpha^{ub}_{ik} = \alpha^u_{ik}, \quad \mathbf{x}\in\Gamma_{ui}, \quad i\in J_p, \tag{25}$$

$$\mathbf{u}_0 = 0, \qquad \mathbf{u}_b = \mathbf{u}_{\Gamma i}, \qquad \mathbf{x}\in\Gamma_{ui}, \qquad \Gamma_{u0}\neq\wedge, \qquad i\in J_r, \tag{26}$$

$$\varphi_0 = \Phi_{0i}, \qquad \varphi_b = \Phi_{bi}, \qquad \Phi_{0i}+\Phi_{bi} = \Phi_i, \qquad \mathbf{x}\in\Gamma_{\varphi i}, \qquad i\in J_Q, \tag{27}$$

$$\varphi_0 = 0, \qquad \varphi_b = V_i, \qquad \mathbf{x}\in\Gamma_{\varphi i}, \qquad \Gamma_{\varphi 0}\neq\wedge, \qquad i\in J_V, \tag{28}$$

and therefore, $\mathbf{u}_0\in H^1_u$, $\varphi_0\in H^1_\varphi$.

By using (24) we can rewrite the system (15), (16) in the form

$$\begin{aligned}&(-\omega^2 + j\omega\alpha_d)\,\rho(\mathbf{v},\mathbf{u}_0) + (-\omega^2 + j\omega\alpha^p_d)\,\rho_P(\mathbf{v},\mathbf{u}_0) +\\ &+(1+j\omega\beta_d)\,c_\Omega(\mathbf{v},\mathbf{u}_0) + (1+j\omega\beta^s_d)\,c_\Gamma(\mathbf{v},\mathbf{u}_0) + e(\varphi_0,\mathbf{v}) = L_u(\mathbf{v}),\end{aligned} \tag{29}$$

$$-e(\chi,\mathbf{u}_0) + (1+j\omega\varsigma_d)^{-1}\kappa_\Omega(\chi,\varphi_0) + (1+j\omega\varsigma^s_d)^{-1}\kappa_\Gamma(\chi,\varphi_0) = L_\varphi(\chi), \tag{30}$$

where

$$\begin{aligned}L_u(\mathbf{v}) = \widetilde{L}_u(\mathbf{v}) &- (-\omega^2 + j\omega\alpha_d)\,\rho(\mathbf{v},\mathbf{u}_b) - (-\omega^2 + j\omega\alpha^p_d)\,\rho_P(\mathbf{v},\mathbf{u}_b) -\\ &-(1+j\omega\beta_d)\,c_\Omega(\mathbf{v},\mathbf{u}_b) - (1+j\omega\beta^s_d)\,c_\Gamma(\mathbf{v},\mathbf{u}_b) - e(\varphi_b,\mathbf{v}),\end{aligned} \tag{31}$$

$$L_\varphi(\chi) = \widetilde{L}_\varphi(\chi) + e(\chi,\mathbf{u}_b) - (1+j\omega\varsigma_d)^{-1}\kappa_\Omega(\chi,\varphi_b) - (1+j\omega\varsigma^s_d)^{-1}\kappa_\Gamma(\chi,\varphi_b). \tag{32}$$

As it can be easily noted, an account for surface effects for piezoelectric bodies in relations (18) – (32) is reduced to adding the forms $c_\Gamma(\mathbf{v},\mathbf{u})$ and $\kappa_\Gamma(\chi,\varphi)$. Therefore we can use the approaches from (Belokon, 1996, 2002, Nasedkin, 2010) for conventional problems for piezoelectric bodies without surface effects.

Now we can define of generalized or weak solution of harmonic problem (1) – (17) using previously introduced functional spaces.

Definition 1. The functions $\mathbf{u}$, φ in the form (24) are the weak solution of harmonic problem for piezoelectric bodies with the generalized Rayleigh damping and with account for surface effects, if Eqs. (29), (30) with (31), (32), (20) – (28) are satisfied for $\forall\ \mathbf{v} \in H_u^1$, $\chi \in H_\varphi^1$.

Let us consider the case $\alpha_d = \alpha_d^p$, $\beta_d = \beta_d^s = \varsigma_d = \varsigma_d^s$ more explicitly.

Then the forms $\widetilde{\rho}(\mathbf{v},\mathbf{u}_0) = \rho(\mathbf{v},\mathbf{u}_0) + \rho_P(\mathbf{v},\mathbf{u}_0)$, $c(\mathbf{v},\mathbf{u}_0) = c_\Omega(\mathbf{v},\mathbf{u}_0) + c_\Gamma(\mathbf{v},\mathbf{u}_0)$, $\kappa(\chi,\varphi_0) = \kappa_\Omega(\chi,\varphi_0) + \kappa_\Gamma(\chi,\varphi_0)$ are symmetrical, bilinear and positive defined in L_2, H_u^1, H_φ^1 respectively, while $e(\varphi_0,\mathbf{v})$ or $e(\chi,\mathbf{u}_0)$ is bilinear form. The forms $e(\chi,\mathbf{u}_0)$, $\kappa(\chi,\varphi_0)$ for fixed $\mathbf{u}_0 \in H_u^1$, $\varphi_0 \in H_\varphi^1$ and $L_\varphi(\chi)$ are linear-bounded functionals in H_φ^1. By Riesz' theorem the elements $e\mathbf{u}_0$, $\kappa\varphi_0$ and l_φ exist and are unique for all $\chi \in H_\varphi^1$.

$$e(\chi,\mathbf{u}_0) = (\chi, e\mathbf{u}_0)_{H_\varphi^1}, \qquad \kappa(\chi,\varphi_0) = (\chi,\kappa\varphi_0)_{H_\varphi^1}, \qquad L_\varphi(\chi) = (\chi, l_\varphi)_{H_\varphi^1}. \tag{33}$$

For variable $\mathbf{u}_0 \in H_u^1$, $\varphi_0 \in H_\varphi^1$ it is obvious that $e\mathbf{u}_0$ and $\kappa\varphi_0$ are linear operators acting from H_u^1 into H_φ^1 and from H_φ^1 into H_φ^1, respectively, and an inverse exists for the operator $\kappa\varphi_0$. Then, from (30), (33) we obtain that

$$\kappa\varphi_0 = (1 + j\omega\beta_d)(e\mathbf{u}_0 + l_\varphi), \quad \varphi_0 = (1 + j\omega\beta_d)(A\mathbf{u}_0 + \kappa^{-1} l_\varphi), \qquad A = \kappa^{-1} e, \tag{34}$$

where the operator A act from H_u^1 into H_φ^1, and is linear and bounded.

Using (33), (34) we can represent the system (29), (30) in the reduced form

$$\begin{aligned} -\omega^2 \widetilde{\rho}(\mathbf{v},\mathbf{u}_0) + j\omega[\alpha_d\, \widetilde{\rho}(\mathbf{v},\mathbf{u}_0) + \beta_d \widetilde{c}(\mathbf{v},\mathbf{u}_0)] + \widetilde{c}(\mathbf{v},\mathbf{u}_0) = \\ = L_u(\mathbf{v}) - (1 + j\omega\beta_d)^{-1} \kappa(\kappa^{-1} l_\varphi, A\mathbf{v}), \end{aligned} \tag{35}$$

where

$$\widetilde{c}(\mathbf{v},\mathbf{u}_0) = c(\mathbf{v},\mathbf{u}_0) + \kappa(A\mathbf{v}, A\mathbf{u}_0). \tag{36}$$

Note that the form $\widetilde{c}(\mathbf{v},\mathbf{u}_0)$ is positive defined in H_u^1, that is provided by conditions (6), (9). So we can introduce the functional space H_c^1 with the scalar product $\widetilde{c}(\mathbf{v},\mathbf{u}_0)$, and this space is equivalent to H_u^1. As is obvious the basic mathematical properties of the problem (35) are the same as for appropriate problems for elastic bodies (Altenbach, 2010).

EIGENVALUE PROBLEM

In this section we focus on eigenvalue problems for piezoelectric solids with account for surface effects. Such problems are central to the analysis of real piezoelectric nanosize devices working in dynamic conditions. Indeed, the frequencies of electric resonances and antiresonances are the natural frequencies of a piezoelectric body. These frequencies determine the dynamic electromechanical coupling factors and the most effective frequency ranges for real piezoelectric nanosize device.

The natural frequencies $f_k = \omega_k / (2\pi)$ for piezoelectric solids can be found from the solution of the generalized eigenvalue problem or modal problem, obtained from (29), (30) with

$\alpha_d = \alpha_d^p = \beta_d = \beta_d^s = \varsigma_d = \varsigma_d^s = 0$, $L_u(\mathbf{v}) = 0$, $L_\varphi(\chi) = 0$, $L_u(\mathbf{v}) = 0$, $L_{\varphi 0}(\chi) = 0$, i.e., without any external inhomogeneous influences and without damping effects (then, $\mathbf{u} = \mathbf{u}_0$, $\varphi = \varphi_0$)

$$-\omega^2 \tilde{\rho}(\mathbf{v},\mathbf{u}) + c(\mathbf{v},\mathbf{u}) + e(\varphi,\mathbf{v}) = 0, \tag{37}$$

$$-e(\chi,\mathbf{u}) + \kappa(\chi,\varphi) = 0, \tag{38}$$

or from (35) we can write the reduced formulation

$$-\omega^2 \tilde{\rho}(\mathbf{v},\mathbf{u}) + \tilde{c}(\mathbf{v},\mathbf{u}) = 0. \tag{39}$$

This eigenvalue problem for the case $\tilde{\rho}(\mathbf{v},\mathbf{u}) = \rho(\mathbf{v},\mathbf{u})$, i.e. without contact boundary conditions, is recently investigated in (Nasedkin, 2013) by using the approaches from (Belokon, 1996, Altenbach, 2011). Because form $\tilde{\rho}(\mathbf{v},\mathbf{u})$ have the same principal mathematical properties that form $\rho(\mathbf{v},\mathbf{u})$, the following principal results take place for eigenvalue problem (37), (38) or (39).

Definition 2. We will call the triple of quantities ω^2, $\mathbf{u} \in H_u^1$, $\varphi \in H_\varphi^1$, which satisfy (39) for arbitrary vector function $\mathbf{v} \in H_u^1$ or, which is equivalent, (37), (38) for arbitrary $\mathbf{v} \in H_u^1$, $\chi \in H_\varphi^1$ a generalized or weak solution of eigenvalue problem (1) – (17) for piezoelectric body with account for surface effects.

Theorem 1. The operator equation (39) of eigenvalue problem for piezoelectric body with account for surface effects has a discrete real spectrum $0 < \omega_1^2 \le \omega_1^2 \le \ldots \le \omega_k^2 \le \ldots$; $\omega_k^2 \to \infty$ as $k \to \infty$, and the corresponding eigenvectors $\mathbf{u}^{(k)}$ form a system that is orthogonal and complete in the spaces H_ρ^0 and H_c^1.

Theorem 2. (The Courant—Fisher minimax principle).

$$\omega_k^2 = \max_{\mathbf{w}_1,\mathbf{w}_2,\ldots,\mathbf{w}_{k-1} \in H_u^1} \left[\min_{\substack{\mathbf{v}\neq 0,\, \mathbf{v}\in H_u^1 \\ \tilde{\rho}(\mathbf{v},\mathbf{w}_j)=0;\; j=1,2,\ldots,k\text{-}1}} R(\mathbf{v}) \right]$$

where $R(\mathbf{v}) = \tilde{c}(\mathbf{v},\mathbf{v}) / \tilde{\rho}(\mathbf{v},\mathbf{v})$ is the Rayleigh quotient.

We observe that the orthogonality conditions in Theorem 1 can be presented in the forms

$$(\mathbf{u}^{(i)},\mathbf{u}^{(j)})_{H_\rho^0} = 0, \qquad (\mathbf{u}^{(i)},\mathbf{u}^{(j)})_{H_c^1} = 0, \qquad i \ne j,$$

and also in the extended writing

$$c(\mathbf{u}^{(i)},\mathbf{u}^{(j)}) + e(\varphi^{(i)},\mathbf{u}^{(j)}) = 0,$$

$$-e(\varphi^{(i)},\mathbf{u}^{(j)}) + \kappa(\varphi^{(i)},\varphi^{(j)}) = 0,$$

where $i \ne j$, $\varphi^{(i)} = A\mathbf{u}^{(i)}$, $\varphi^{(j)} = A\mathbf{u}^{(j)}$.

Also in (Nasedkin, 2013) a number of theorems that establish the dependencies of eigenfrequencies of piezoelectric nanodimensional bodies were formulated with account for surface stresses and dielectric films and with the change of the mechanical and electric boundary conditions and material parameters.

Thus, the following theorems hold.

Theorem 3. The natural frequencies ω_k for the eigenvalue problem with account for surface stresses are not less than the corresponding natural frequencies $\omega_{f\,uk}$ for the problem without account for surface stresses, i.e. $\omega^2_{f\,uk} \le \omega^2_k$ for $\forall\ k$.

Theorem 4. The natural frequencies ω_k for the eigenvalue problem with account for surface electric charges are not greater than the corresponding natural frequencies $\omega_{f\,\varphi k}$ for the problem without account for surface electric charges, i.e. $\omega^2_k \le \omega^2_{f\,\varphi k}$ for $\forall\ k$.

In (Belokon, 1996, Nasedkin, 2013) we also investigate the natural frequencies under the changes of certain parameters of the problem. For the next theorems we will explicitly point these changes in the formulations of the theorems, and all the variables related to the modified problems will be marked by subscripts lm or by an asterisk. As above, for the initial and modified problems the parameters that are not specified in the theorem formulations are assumed to be identical.

We will call problem (37), (38) or (39), the lm-problem, emphasizing by this the presence of l areas Γ_{ui}, $i \in J_p = \{1, 2, ..., l\}$ in contact with rigid plane punches and m open-circuited electrodes $\Gamma_{\varphi i}$, $i \in J_Q = \{1, 2, ..., m\}$.

We will consider two similar lm- and pm-problems, which differ solely in the number l and p of contacting surfaces of Γ_{ui} in (10) – (12). All the remaining input data from (1) – (17) in the lm- and pm-problems are assumed to be the same.

Theorem 5. If $0 \le l \le p \le L$, then the *k*th natural frequency ω_{lmk} of lm-problem is no less than *k*th natural frequency ω_{pmk} of pm-problem, i.e. $\omega^2_{lmk} \ge \omega^2_{pmk}$ for $\forall\ k$.

Note that in conditions of Theorem 5, we do not change the boundary Γ_u. When passing from *lm*-problem to *pm*-problem, we change only the conditions of fixed boundary to the conditions of contact with punches on the parts of Γ_{ui}.

We now consider two similar lm- and ln-problems, which differ solely in the number m and n of open-circuited electrodes of $\Gamma_{\varphi i}$ in (15) – (17).

Theorem 6. If $0 \le m \le n \le M$, then the *k*th natural frequency ω_{lmk} of the lm-problem is no greater than the *k*th natural frequency ω_{lnk} of the *ln*-problem, i.e. $\omega^2_{lmk} \le \omega^2_{lnk}$ for $\forall\ k$.

For the next theorems we missing the subscripts lm, because for two compare problems the collections of elements in $J_p = \{1, 2, ..., l\}$ and $J_Q = \{1, 2, ..., m\}$ are the same.

Theorem 7. If for two problems the rigid fixed boundaries and the boundaries, contacting with the punches, are such that $\Gamma_u \supseteq \Gamma_{*u}$, $\Gamma_{ui} \supseteq \Gamma_{*ui}$, $i = 0, 1, 2, ..., L$, then we have $\omega^2_k \ge \omega^2_{*k}$ for $\forall\ k$.

Theorem 8. If for two problems the elastic moduli, the piezomoduli, the densities of piezoelectric material and the inertia moments of the punches are such that $\tilde{c}(\mathbf{v},\mathbf{v}) \geq \tilde{c}_*(\mathbf{v},\mathbf{v})$, $\tilde{\rho}(\mathbf{v},\mathbf{v}) \leq \tilde{\rho}_*(\mathbf{v},\mathbf{v})$ for $\forall\ \mathbf{v} \in H_u^1$, then $\omega_k^2 \geq \omega_{*k}^2$ for $\forall\ k$.

Theorem 9. If the electrode boundaries of two problems are such that $\Gamma_\varphi \supseteq \Gamma_{*\varphi}$, $\Gamma_{\varphi i} \supseteq \Gamma_{*\varphi i}$, $i = 0,1,2,...,M$, then we have $\omega_k^2 \leq \omega_{*k}^2$ for $\forall\ k$.

Theorem 10. If the permittivities of two problems are such that $\kappa(\chi,\chi) \geq \kappa_*(\chi,\chi)$ for $\forall\ \chi \in H_\varphi^1$, then $\omega_k^2 \leq \omega_{*k}^2$ for $\forall\ k$.

Now we will summarize the results of Theorems 5 – 10.

If on certain areas of Γ_{ui} we replace the boundary conditions of rigid clamping (13) by the contact boundary conditions (10)–(12), then, by Theorem 5, the natural frequencies can only decrease.

On the other hand, if on certain areas of $\Gamma_{\varphi i}$ we replace the boundary conditions for the electric potential of zero (17) with electric boundary conditions of contact type (15), (16) for open-circuited electrodes, then by Theorem 6 the natural frequencies can only increase.

Note that the natural frequencies in the problem with all operation short-circuited electrodes are usually named as electric resonance frequencies, while the natural frequencies in the problem with some open-circuited electrodes are usually named as electric antiresonance frequencies. Therefore, Theorem 6 also asserts that *electric antiresonance frequencies are not less than the electric resonance frequencies with the same order numbers*.

By Theorems 7 and 8, a reduction in the boundaries Γ_{ui} or a specific reduction in the elastic moduli and an increase in the density or in the massive characteristics of punches can lead only to a decrease in the natural frequencies.

Conversely, by Theorems 9 and 10, a reduction in the electrode boundary $\Gamma_{\varphi i}$ or a specific reduction in the permittivity moduli can lead only to an increase in the natural frequencies.

We note that the results of theorems 5 – 10 are valid for both problems with and without account for surface effects.

Comparing the effects reflected in Theorems 3, 5, 7, 8 and 4, 6, 9, 10, we can conclude that a similar change in the mechanical and electric boundary conditions or in elastic and permittivity moduli leads to an opposite change in the natural frequencies.

FINITE ELEMENT APPROXIMATIONS

For numerical solution of the harmonic problems (29), (30) (or of the eigenvalue problems) we can use classical technique of finite element analysis. Let Ω_h be the region occupied by the corresponding finite element mesh $\Omega_h \subseteq \Omega$, $\Omega_h = \cup_k \Omega^{ek}$, where Ω^{ek} is separate finite element with number k. At the boundary $\Gamma_h = \partial\Omega_h$ we select the regions $\Gamma_{h\sigma}$, Γ_{hui}, $i = 0,1,2,...,L$, Γ_{hD}, $\Gamma_{h\varphi i}$, $i = 0,1,2,...,M$, that approximate the corresponding boundaries Γ_σ, Γ_{ui}, Γ_D, $\Gamma_{\varphi i}$. Then on Ω_h the finite functional spaces H_{hu}^1, $H_{h\varphi}^1$ can be introduced analogously to spaces H_u^1, H_φ^1.

We will search the approximate solution $\mathbf{u}_{h0} \approx \mathbf{u}_0$, $\varphi_{h0} \approx \varphi_0$ of the problem (29), (30) on the finite element mesh $\Omega_h = \cup_k \Omega^{ek}$ in the form

$$\mathbf{u}_{h0}(\mathbf{x}) = \mathbf{N}_u^T \cdot \mathbf{U}, \qquad \varphi_{h0}(\mathbf{x}) = \mathbf{N}_\varphi^T \cdot \mathbf{\Phi}, \tag{40}$$

where $\mathbf{N}_u^T$ is the matrix of the form functions (basis functions) for the displacements, $\mathbf{N}_\varphi^T$ is the row vector of the form functions for electric potential, $\mathbf{U}$, $\mathbf{\Phi}$ are the global vectors of nodal values for displacements and electric potential, respectively.

The projection functions $\mathbf{v} \in H_u^1$, $\chi \in H_\varphi^1$ can be presented in the form

$$\mathbf{v}(\mathbf{x}) = \mathbf{N}_u^T \cdot \delta\mathbf{U}, \qquad \chi(\mathbf{x}) = \mathbf{N}_\varphi^T \cdot \delta\mathbf{\Phi}. \tag{41}$$

According to the conventional finite element technique we will write the weak setting of the problem (29), (30) in finite spaces H_{hu}^1 и $H_{h\varphi}^1$ for the region $\Omega_h = \cup_k \Omega^{ek}$ with corresponding boundaries. Substituting (40), (41) in the problem (29), (30) for Ω_h, we will have

$$[(-\omega^2 + j\omega\alpha_d)\mathbf{M}_{uu} + (-\omega^2 + j\omega\alpha_d^p)\mathbf{M}_{Puu} + (1 + j\omega\beta_d)\mathbf{K}_{\Omega uu} + (1 + j\omega\beta_d^s)\mathbf{K}_{\Gamma uu}] \cdot \mathbf{U} + \mathbf{K}_{u\varphi} \cdot \mathbf{\Phi} = \mathbf{F}_u \tag{42}$$

$$-\mathbf{K}_{u\varphi}^T \cdot \mathbf{U} + [(1 + j\omega\varsigma_d)^{-1}\mathbf{K}_{\Omega\varphi\varphi} + (1 + j\omega\varsigma_d^s)^{-1}\mathbf{K}_{\Gamma\varphi\varphi}] \cdot \mathbf{\Phi} = \mathbf{F}_\varphi, \tag{43}$$

where $\mathbf{M}_{uu} = \sum_k^a \mathbf{M}_{uu}^{ek}$, $\mathbf{K}_{\Omega uu} = \sum_k^a \mathbf{K}_{\Omega uu}^{ek}$, $\mathbf{K}_{\Gamma uu} = \sum_k^a \mathbf{K}_{\Gamma uu}^{ek}$, $\mathbf{K}_{u\varphi} = \sum_k^a \mathbf{K}_{u\varphi}^{ek}$, $\mathbf{K}_{\Omega\varphi\varphi} = \sum_k^a \mathbf{K}_{\Omega\varphi\varphi}^{ek}$, $\mathbf{K}_{\Gamma\varphi\varphi} = \sum_k^a \mathbf{K}_{\Gamma\varphi\varphi}^{ek}$ are the global finite element matrices obtained from the corresponding element matrices as the result of the assembly procedure ($\sum_k^a$), and $\mathbf{M}_{Puu}$ is the matrix of punch mass and inertia characteristics.

According to (20)–(23), the element matrices are in the following form

$$\mathbf{M}_{uu}^{ek} = \int_{\Omega^{ek}} \rho \mathbf{N}_u^e \cdot \mathbf{N}_u^{eT} d\Omega, \quad \mathbf{K}_{\Omega uu}^{ek} = \int_{\Omega^{ek}} \mathbf{B}_u^{eT} \cdot \mathbf{c} \cdot \mathbf{B}_u^e d\Omega, \quad \mathbf{K}_{\Gamma uu}^{ek} = \int_{\Gamma_\tau^{ek}} \mathbf{B}_{su}^{eT} \cdot \mathbf{c}^s \cdot \mathbf{B}_{su}^e d\Omega, \tag{44}$$

$$\mathbf{K}_{u\varphi}^{ek} = \int_{\Omega^{ek}} \mathbf{B}_u^{eT} \cdot \mathbf{e}^T \cdot \mathbf{B}_\varphi^e d\Omega, \quad \mathbf{K}_{\Omega\varphi\varphi}^{ek} = \int_{\Omega^{ek}} \mathbf{B}_\varphi^{eT} \cdot \boldsymbol{\kappa} \cdot \mathbf{B}_\varphi^e d\Omega, \quad \mathbf{K}_{\Gamma\varphi\varphi}^{ek} = \int_{\Gamma_D^{ek}} \mathbf{B}_{s\varphi}^{eT} \cdot \boldsymbol{\kappa}^s \cdot \mathbf{B}_{s\varphi}^e d\Omega, \tag{45}$$

$$\mathbf{B}_{(s)u}^e = \mathbf{L}(\nabla^{(s)}) \cdot \mathbf{N}_u^{eT}, \qquad \mathbf{B}_{(s)\varphi}^e = \nabla^{(s)} \mathbf{N}_\varphi^{eT}, \tag{46}$$

$$\mathbf{L}^T(\nabla^{(s)}) = \begin{bmatrix} \partial_1^{(s)} & 0 & 0 & 0 & \partial_3^{(s)} & \partial_2^{(s)} \\ 0 & \partial_2^{(s)} & 0 & \partial_3^{(s)} & 0 & \partial_1^{(s)} \\ 0 & 0 & \partial_3^{(s)} & \partial_2^{(s)} & \partial_1^{(s)} & 0 \end{bmatrix}, \qquad \partial_i^{(s)} = \partial_i - n_i \frac{\partial}{\partial r}, \qquad i = 1, 2, 3, \tag{47}$$

where Γ_τ^{ek}, Γ_D^{ek} are the edges of finite elements facing the regions $\Gamma_{h\tau}$, Γ_{hD} with given surface effects, $\mathbf{N}_u^{eT}$, $\mathbf{N}_\varphi^{eT}$ are the matrices and row vectors of approximating basis functions, respectively, that are defined at separate finite elements.

In (44) – (47) we used matrix-vector notations: $\mathbf{c}$, $\mathbf{c}^s$ are 6x6 matrices of elastic stiffness bulk and surface modules, $c_{\alpha\beta}^{(s)} = c_{ijkl}^{(s)}$; $\mathbf{e}$ is 3x6 matrix of piezomoduli, $e_{i\beta} = e_{ikl}$; $\alpha, \beta = 1, ..., 6$;

$i, j, k, l = 1, 2, 3$ with the correspondence law $\alpha \leftrightarrow (i\,j)$, $\beta \leftrightarrow (k\,l)$, $1 \leftrightarrow (11)$, $2 \leftrightarrow (22)$, $3 \leftrightarrow (33)$, $4 \leftrightarrow (23) = (32)$, $5 \leftrightarrow (13) = (31)$, $6 \leftrightarrow (12) = (21)$.

We note that in (42) – (47) the global and element matrices of mass and stiffness $\mathbf{M}_{uu}$, $\mathbf{M}_{uu}^{ek}$, $\mathbf{K}_{\Omega uu}$, $\mathbf{K}_{\Omega uu}^{ek}$ and nodal force vector $\mathbf{F}_u$ are formed in the same way as for purely elastic body, and the matrices $\mathbf{K}_{u\varphi}$, $\mathbf{K}_{u\varphi}^{ek}$, $\mathbf{K}_{\Omega\varphi\varphi}$, $\mathbf{K}_{\Omega\varphi\varphi}^{ek}$ and nodal force vector $\mathbf{F}_\varphi$ are identical to the corresponding matrices and vector for piezoelectric bodies. The matrices $\mathbf{K}_{\Gamma uu}$, $\mathbf{K}_{\Gamma uu}^{ek}$ and $\mathbf{K}_{\Gamma\varphi\varphi}$, $\mathbf{K}_{\Gamma\varphi\varphi}^{ek}$ are defined by the surface stresses and surface electric charges, respectively. These matrices are analogous to the stiffness matrices for surface elastic membranes and the matrices of dielectric permittivities for surface dielectric films. Hence, for implementing the finite element piezoelectric analysis for the bodies with surface effects it is necessary to have surface structural membrane elements and surface finite elements of dielectric films along with ordinary solid piezoelectric finite elements.

We can conclude that the harmonic and modal analysis technique for the piezoelectric bodies with surface effects can repeat similar technique for piezoelectric bodies without surface effects. In particular, the same solvers for eigenvalue problems can be used to determine practically important frequencies of electric resonances and antiresonances (see for example (Iovane, 2010)).

Thus, for modal analysis with $\alpha_d = \alpha_d^p = \beta_d = \beta_d^s = \varsigma_d = \varsigma_d^s = 0$, $\mathbf{F}_u = 0$, $\mathbf{F}_\varphi = 0$, the system (42), (43) is the generalized eigenvalue problem

$$\mathbf{K}_{uu} \cdot \mathbf{U} + \mathbf{K}_{u\varphi} \cdot \mathbf{\Phi} = \omega^2 \widetilde{\mathbf{M}}_{uu} \cdot \mathbf{U}, \tag{48}$$

$$-\mathbf{K}_{u\varphi}^T \cdot \mathbf{U} + \mathbf{K}_{\varphi\varphi} \cdot \mathbf{\Phi} = 0, \tag{49}$$

where

$$\widetilde{\mathbf{M}}_{uu} = \mathbf{M}_{uu} + \mathbf{M}_{Puu}, \quad \mathbf{K}_{uu} = \mathbf{K}_{\Omega uu} + \mathbf{K}_{\Gamma uu}, \quad \mathbf{K}_{\varphi\varphi} = \mathbf{K}_{\Omega\varphi\varphi} + \mathbf{K}_{\Gamma\varphi\varphi}.$$

Eigenvalue problem (48), (49) can be represented in the form

$$\widetilde{\mathbf{K}}_{uu} \cdot \mathbf{U} = \lambda \widetilde{\mathbf{M}}_{uu} \cdot \mathbf{U}, \quad \lambda = \omega^2,$$

where

$$\widetilde{\mathbf{K}}_{uu} = \mathbf{K}_{uu} + \mathbf{K}_{u\varphi} \cdot \mathbf{K}_{\varphi\varphi}^{-1} \cdot \mathbf{K}_{u\varphi}^T.$$

It is obvious, that the generalized stiffness matrix $\widetilde{\mathbf{K}}_{uu}$ and the total mass matrix $\widetilde{\mathbf{M}}_{uu}$ are positive defined ($\widetilde{\mathbf{K}}_{uu} > 0$, $\widetilde{\mathbf{M}}_{uu} > 0$). Then, the eigenvalues $\lambda_k = \omega_k^2$ ($k = 1, 2, ..., n; n$ is the order of matrices $\widetilde{\mathbf{K}}_{uu}$ and $\widetilde{\mathbf{M}}_{uu}$) are real and positive. The eigenvectors, corresponding to them, which we will denote by $\mathbf{W}_k$, form basis in R^n. The system of these eigenvectors $\mathbf{W}_k$ can be chosen orthonormal with respect to the total mass matrix $\widetilde{\mathbf{M}}_{uu}$ and orthogonal with respect to the generalized stiffness matrix $\widetilde{\mathbf{K}}_{uu}$

$$\mathbf{W}_k^T \cdot \widetilde{\mathbf{M}}_{uu} \cdot \mathbf{W}_m = \delta_{km}, \qquad \mathbf{W}_k^T \cdot \widetilde{\mathbf{K}}_{uu} \cdot \mathbf{W}_m = \omega_m^2 \delta_{km}. \tag{50}$$

Note that the indicated properties of eigenvalues and eigenvectors are the discrete variants of the corresponding continual properties established in Theorem 1.

By using the orthogonality relations (50) we can apply the mode superposition method for solution of harmonic problem for the more important case $\alpha_d = \alpha_d^p$, $\beta_d = \beta_d^s = \varsigma_d = \varsigma_d^s$. For such values of damping coefficients the system of finite element equations has the following structure

$$[(-\omega^2 + j\omega\alpha_d)\tilde{\mathbf{M}}_{uu} + (1 + j\omega\beta_d)\mathbf{K}_{uu}] \cdot \mathbf{U} + \mathbf{K}_{u\varphi} \cdot \mathbf{\Phi} = \mathbf{F}_u ,$$

$$-\mathbf{K}_{u\varphi}^T \cdot \mathbf{U} + (1 + j\omega\beta_d)^{-1}\mathbf{K}_{\varphi\varphi} \cdot \mathbf{\Phi} = \mathbf{F}_\varphi ,$$

or, in the reduced form

$$[-\omega^2\tilde{\mathbf{M}}_{uu} + j\omega\tilde{\mathbf{C}}_{uu} + \tilde{\mathbf{K}}_{uu}] \cdot \mathbf{U} = \tilde{\mathbf{F}}_u , \tag{51}$$

$$\mathbf{\Phi} = (1 + j\omega\beta_d)\mathbf{K}_{\varphi\varphi}^{-1} \cdot (\mathbf{K}_{u\varphi}^T \cdot \mathbf{U} + \mathbf{F}_\varphi) , \tag{52}$$

where $\tilde{\mathbf{C}}_{uu} = \alpha_d\tilde{\mathbf{M}}_{uu} + \beta_d\tilde{\mathbf{K}}_{uu}$, $\tilde{\mathbf{F}}_u = \mathbf{F}_u - (1 + j\omega\beta_d)\mathbf{K}_{u\varphi} \cdot \mathbf{K}_{\varphi\varphi}^{-1} \cdot \mathbf{F}_\varphi$.

Thus, we will find the solution of problem (51) in the form of an expansion in eigenvectors (modes) $\mathbf{W}_k$ of eigenvalue problem (48), (49)

$$\mathbf{U} = \sum\nolimits_{k=1}^{n} z_k \mathbf{W}_k . \tag{53}$$

Substituting (53) into (51) and multiplying the obtained equation scalarly by $\mathbf{W}_m^T$ and taking into account the orthogonality relations (50), we obtain

$$z_k = \frac{1}{\omega_k^2 - \omega^2 + 2j\xi_k\omega\omega_k} P_k , \quad P_k = \mathbf{W}_k^T \cdot \tilde{\mathbf{F}}_u , \quad \xi_k = \alpha_d \frac{1}{2\omega_k} + \beta_d \frac{\omega_k}{2} . \tag{54}$$

Thus, using the method of mode superposition, the solutions of the harmonic problems are determined by (53), (54) and (52).

The advantages and disadvantages of the mode superposition method are well known from experience of solving problems of structural analysis. Consequently, an important advantage of the method is the possibility of a direct determination of the damping coefficient ξ_k of the individual modes without using the last formula from (54). These factors can be specified from the experimentally measured value of the mechanical quality factor Q_k of the mode with number k: $\xi_k = 1/(2Q_k)$.

NUMERICAL RESULTS

As an example we consider the problem of natural oscillations of a longitudinally polarized piezoelectric rod with a circular cross-section made of zinc oxide (*ZnO*). We adopt that the rod has the length $l = 1 \cdot 10^{-6}$ (m) and the radius $R = 0.05 \cdot 10^{-6}$ (m). For zinc oxide (which is *6mm*-class material) we set the following bulk moduli (Dieulesaint, 1974): $\rho = 5.676 \cdot 10^3$, $c_{11}^E = 2.097 \cdot 10^{11}$, $c_{12}^E = 1.211 \cdot 10^{11}$, $c_{13}^E = 1.051 \cdot 10^{11}$, $c_{33}^E = 2.109 \cdot 10^{11}$, $c_{44}^E = 0.425 \cdot 10^{11}$ (N/m^2), $e_{31} = -0.61$, $e_{33} = 1.14$, $e_{15} = -0.59$ (Cl/m^2), $\varepsilon_{11}^S = 7.38\varepsilon_0$, $\varepsilon_{33}^S = 7.83\varepsilon_0$, $\varepsilon_0 = 8.85 \cdot 10^{-12}$

(F/m). We refer the rod to the cylindrical coordinate system $Or\theta z$, directing z -axis along the symmetry axis of the rod and choosing the coordinate system origin to lay in the plane of the lower end of the rod. We will assume that the ends of the rod $z=l$ and $z=0$ are covered with electrodes, for the upper electrode $\varphi = V_0$ (i.e., $V_0 \exp(j\omega t)$), and for the lower electrode $\varphi = 0$ in the harmonic problem. For determination of the electric resonance frequencies f_{rk} ($f = \omega/(2\pi)$) from the eigenvalue problem, we assume that $V_0 = 0$. Here, on the upper electrode $z=l$ the boundary conditions (15), (16) with $Q_1 = 0$ are satisfied for the eigenvalue problem of determination of the electric antiresonance frequencies f_{ak}. The lower end of the rod $z=0$ is considered to be rigidly fixed, and the upper end $z=l$ is covered by rigid punch with mass $M_0^{(1)} = \pi\rho l R^2/2$. We will also assume that the lateral surface $r=R$, $0 \le z \le l$ is the surface $\Gamma_\sigma = \Gamma_D$ with $\mathbf{p}_\Gamma = 0$, $q_\Gamma = 0$ in (7), (14), respectively.

In order to illustrate theorems 3 and 8 let us compare the first two frequencies of electric resonance and antiresonance at the absence and the presence of the surface stresses and under the increase of the stiffness modules of the surface membrane that define the surface stresses. For both eigenvalue problems we do not take into account the effect of the dielectric films.

These and further problems on the natural frequencies will be solved as axisymmetric problems using ANSYS finite element software. We divide the meridian section of the rod into quadrilateral eight-node finite elements PLANE13 with the options for axisymmetric piezoelectric analysis. Let us choose the number of finite elements along the radius to be equal to 30, and along the rod length to be equal to 600. We note that, as the computations have shown, such sufficiently fine mesh provided enough accuracy of the computations under different variations of the input parameters in all the examples considered. To model surface stresses on the lateral surface Γ_σ we place axisymmetric elastic shell finite elements SHELL208 with options of only membrane stresses. Such membrane elements will approximate the boundary conditions (7) with the constitutive equations (8) with appropriate choice of elastic modules of membrane and its thickness. If we adopt that the surface elastic modules $\mathbf{c}^s$ are the elastic modules of isotropic body, than it is enough to set only the surface elastic Young's module E_s and surface Poisson's ratio ν_s. Then for equivalent elastic membrane and the corresponding membrane finite elements in ANSYS finite element package it is necessary to set the Young's module of the membrane E_m, the Poisson's ratio of the membrane ν_m and the thickness of the membrane h_m so that the equalities $E_s = h_m E_m$, $\nu_s = \nu_m$ take place. Therefore, for the equivalent membrane the values E_m and h_m are not significant separately but in their multiplication $E_s = h_m E_m$. Formally putting $h_m = l$, we will set the surface Young's module E_s in the form $E_s = h_m E_m$, $E_m = k_s E_0$, varying the proportion ratio k_s. For the computations we set that $E_0 = 2 \cdot 10^{11}$ (N/m^2), $\nu_s = 0.3$.

We note that to insure the accuracy of the finite element computations in ANSYS due to the smallness of the geometric sizes of the rod here it is convenient to transfer to dimensionless coordinates and parameters that can be introduce as following: $\tilde{\mathbf{u}} = \mathbf{u}/l$, $\tilde{\mathbf{x}} = \mathbf{x}/l$, $\tilde{\varphi} = \varphi/(E_d l)$, $\tilde{\mathbf{c}}^E = \mathbf{c}^E / c_{33}^E$, $\tilde{\mathbf{e}} = \mathbf{e} E_d / c_{33}^E$, $\tilde{\boldsymbol{\varepsilon}}^S = \boldsymbol{\varepsilon}^S / \varepsilon_{11}^S$, $\tilde{\boldsymbol{\sigma}} = \boldsymbol{\sigma} / c_{33}^E$, $\tilde{\mathbf{E}} = \mathbf{E}/E_d$, $\tilde{\mathbf{D}} = \mathbf{D} E_d / c_{33}^E$, $\tilde{\omega} = \omega T_d$, $\tilde{M}_0^{(1)} = M_0^{(1)}/(\rho l^3)$, $T_d = l / v_3^E$, $v_3^E = \sqrt{c_{33}^E/\rho}$, $E_d = \sqrt{c_{33}^E / \varepsilon_{11}^S}$. Then the problem can be solved in dimensionless form for the variables marked with symbol "tilde", and after solving this problem we can return to dimensional quantities.

Fig. 3 (a) illustrates the graphs of the dependencies of the first two electric resonance frequencies f_{r1} and f_{r2} on the coefficient k_s, plotted on the *x*-axis in a logarithmic scale, i.e. at $k_s = 0 = 10^{-\infty}$, 10^{-6}, 10^{-4}, 10^{-2}, etc. As it follows from theorems 3, 8, under the increase of elastic stiffnesses of the surface member the natural frequencies also increase, and they increase considerable at $k_s \geq 10^{-2}$. If along with the electric resonance frequencies we find the electric antiresonance frequencies f_{a1} and f_{a2}, then we can find dynamic frequency coefficients of electromechanical coupling by formulas $k_{d\,i} = \sqrt{1-(f_{r\,i}/f_{a\,i})^2}$, $i = 1, 2$. These coefficients are responsible for electric activity of the corresponding oscillation modes and for effectiveness of the mechanical and electric energy transformation. The corresponding graphs of the Dependence of the electromechanical coupling coefficients $k_{d\,i}$ on k_s are shown in Fig. 3 (b).

As it can be seen, for the example considered the electromechanical coupling coefficient k_{d1} decreases with the increase of the value of surface stiffness, also more considerably at $k_s \geq 10^{-2}$. This property is quite expected for the example considered, but in general it does not follow from the established theorems and for other problems and oscillation modes can not take place, as for example for coupling coefficient k_{d2}.

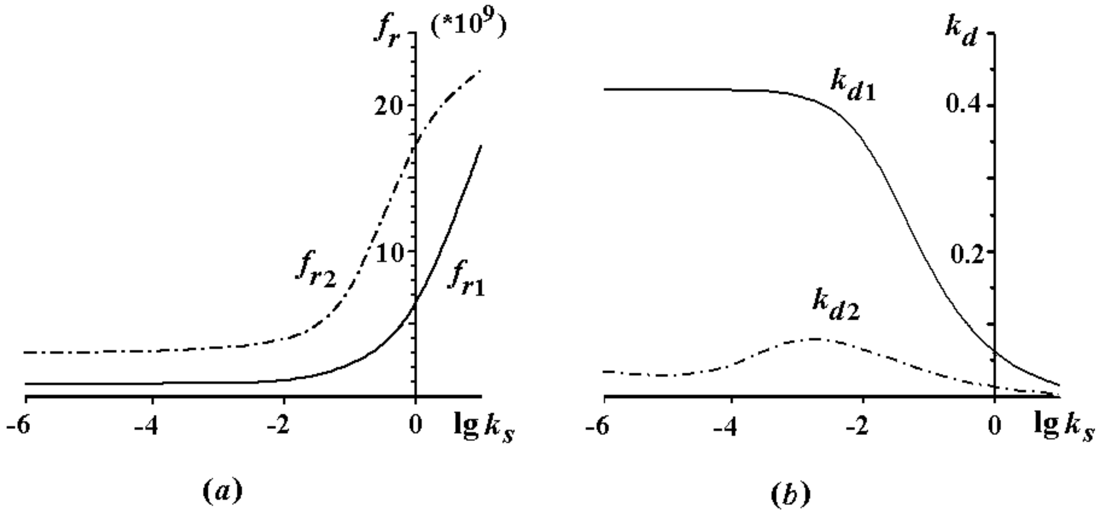

Fig. 3. Resonance frequencies $f_{r\,i}$ (a) and coupling coefficients $k_{d\,i}$ (b) vs. stiffness coefficient k_s.

Account of surface charges and dielectric films is illustrated by Fig. 4 for the problems without surface stresses. Here for computations the simulation of the dielectric film was implemented by adding to the edge $r = R$, $0 \leq z \leq l$ the dielectric layer consisting of finite elements PLANE13 with options of axisymmetric piezoelectric analysis at negligibly small elastic stiffnesses and piezomoduli. Basic dielectric permittivities of three-dimensional dielectric layer were set as follows: $\varepsilon^v_{011} = 0$, $\varepsilon^v_{022} = 7.38\varepsilon_0$, $\varepsilon^v_{033} = 7.83\varepsilon_0$ (F/m). Therefore, basic dielectric permittivities along the radial axis (axis 1) were set to be zero and the other values coincided with the dielectric permittivities of the material *ZnO*. Thickness h_f of the dielectric layer was assumed to be equal to $1 \cdot 10^{-8}$ (m). Such layer simulates the dielectric film and boundary conditions (14) with surface dielectric permittivities $\varepsilon_{ii}^s = h_f \varepsilon_{ii}^v$, $i = 1, 2, 3$ when $\varepsilon_{ii}^v = k_f\, \varepsilon_{0ii}^v$, $k_f = 1$. Further in numerical computations the multiplier k_f was being changed from 0 to 10^4, and accordingly the dielectric permittivities ε_{ii}^v were being changed. The results of the computations are shown in Fig. 4, where Fig. 4 (a) illustrated the graphs of the dependencies of the first two electric resonance frequencies f_{r1} and f_{r2} on coefficient k_f, plotted along the horizontal axis in logarithmic scale, and Fig. 4 (b) illustrated the graphs of the dependency of the electromechanical coupling coefficients $k_{d\,i}$ on k_f. As it follows from theorems 4, 10, with the increase of dielectric permittivities of surface film the natural frequencies decrease. A small decrease of the resonance frequencies can be explained by small dielectric permittivity coefficients and small piezomoduli for piezoelectric material zinc oxide *ZnO*. As it is seen from Fig. 4 (b), for the example considered the electromechanical coupling coefficients decrease with the increase of the variable k_f faster than the resonance frequencies.

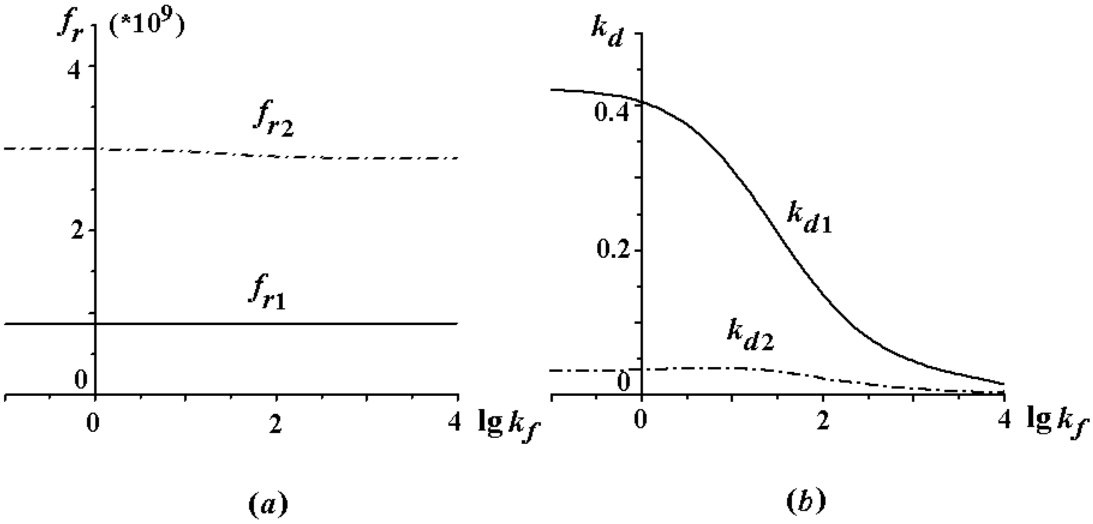

Fig. 4. Resonance frequencies f_{ri} (a) and coupling coefficients $k_{d\,i}$ (b) vs. permittivity coefficient k_f.

Note that similar results and the results illustrating the effect of the mechanical and electrical boundary conditions for the eigenvalue problem for nanodimensional rod without a rigid punch are presented in (Nasedkin, 2013).

We can obtain the analogous results from solution of harmonic problem. For example, Fig. 5 demonstrates the electric admittance $Y = j2\pi f Q_0 / V_0$, $V_0 = 1$ (V) versus frequency near first resonance frequency for considered piezoelectric rod at the absence and the presence of the surface stresses. For this case we assume the following frequency-independent damping properties: $\alpha_d = \alpha_d^p = 0$, $\varsigma_d = \varsigma_d^s = 0$, $\beta_d = \beta_d^s = \xi_d /(\pi f)$, $\xi_d = 1.25 \cdot 10^{-3}$. The hard curve (1) in Fig. 5 corresponds to magnitude of admittance for the road without surface stresses, and the dashed curve (2) is related to magnitude of admittance for the road with surface stresses when $k_s = 10^{-2}$. It can easily be seen from Fig. 5 that the resonance frequencies (maximum $|Y|$) and the antiresonance frequencies (minimum $|Y|$) correspond to similar results, obtained from the solution of eigenvalue problem (Fig. 3 (a) for the same values of k_s).

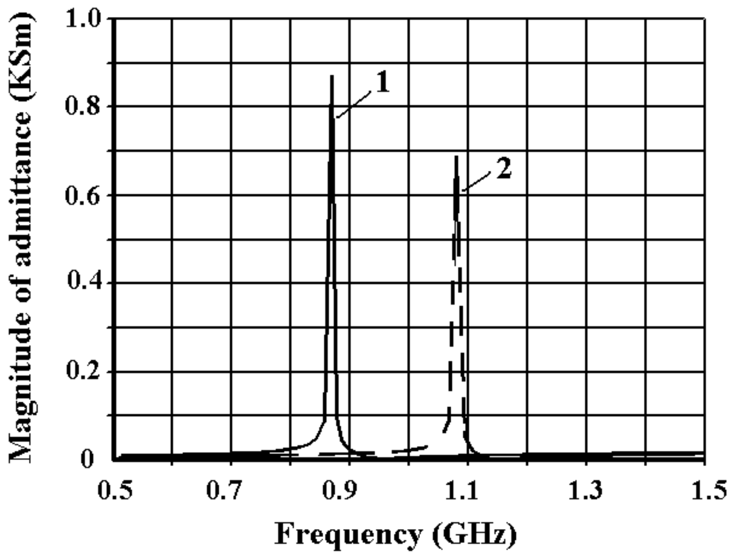

Fig. 5. Magnitude of electric admittance vs. frequency.

CONCLUSION

This paper has considered the harmonic and eigenvalue problems for piezoelectric nanodimensional bodies in the framework of the linear piezoelasticity theory with damping properties and with account for surface effects induced by surface stresses and surface dielectric films.

Classical and generalized settings of the harmonic problems for piezoelectric nanodimensional bodies with damping properties, boundary conditions of contact type and surface effects were formulated in expanded and reduced forms. For generalized settings the corresponding functional spaces were introduced. It was proved that the spectrum for the eigenvalue problem was discrete and real and the eigenvectors were orthogonal.

The theorems that establish the dependencies of natural frequencies were formulated with account for surface stresses and surface dielectric films, and the change of the rigidly fixed boundaries, boundaries of contact type, boundaries with electrodes and material parameters of piezoelectric nanosize bodies.

It was noted that the same changes of mechanical and electric boundary conditions and changes of stiffness characteristics and dielectric permittivities lead to the opposite changes in the natural frequencies. All dependencies were established for the piezoelectric bodies without surface effects, as well as for the bodies with account for surface stresses and surface dielectric films.

Finite element approximations and the corresponding generalized matrix problems were suggested for numerical solution of the harmonic and spectral problems for piezoelectric bodies with surface effects. The results were illustrated with a numerical example for obtaining the natural frequencies and harmonic vibrations of nanosize piezoelectric rod made of zinc oxide under different varied parameters of the problem. It was shown that here standard finite element software could be used with additional introduction of surface membrane elements and surface dielectric films in the computation models.

ACKNOWLEDGMENTS

This work is supported by the Russian Foundation for the Basic Research (12-01-00829).

REFERENCES

Altenbach H, Eremeyev VA, Lebedev LP. On the existence of solution in the linear elasticity with surface stresses. Z. Angew. Math. Mech., 2010, 90(3), p. 231-240.

Altenbach H, Eremeyev VA, Lebedev LP. On the spectrum and stiffness of an elastic body with surface stresses. Z. Angew. Math. Mech., 2011, 91(9), p. 699-710.

Belokon AV, Nasedkin AV, Soloviev AN. New schemes for the finite-element dynamic analysis of piezoelectric devices. J. Applied Math. Mech. (PMM), 2002, 66(3), p. 481-490.

Dieulesaint E, Royer D. Ondes elastiques dans les solides. Application au traitement du signal. Masson, 1974.

Duan HL, Wang J, Huang ZP, Karihaloo BL. Size-dependent effective elastic constants of solids containing nano-inhomogeneities with interface stress. J. Mech. Phys. Solids, 2005, 53, p. 1574-1596.

Duan HL, Wang J, Karihaloo BL, Huang ZP. Nanoporous materials can be made stiffer than non-porous counterparts by surface modification. Acta mater, 2006, 54, p. 2983-2990.

Iovane G, Nasedkin AV. Modal analysis of piezoelectric bodies with voids. II. Finite element simulation. Applied Mathematical Modelling, 2010, 34(1), p. 47-59.

Jing GY, Duan HL, Sun XM et al. Surface effects on elastic properties of silver nanowires: contact atomic-force microscopy. Phys. Rev. B., 2006, 73, p. 235409-1-6.

Nasedkin AV. Some finite element methods and algorithms for solving acousto-piezoelectric problems. In: Parinov IA (ed) Piezoceramic materials and devices. Nova Science Publishers, NY, 2010, p. 177-218.

Nasedkin AV, Eremeyev VA. Spectral properties of piezoelectric bodies with surface effects. In: Altenbach H, Morozov NF (eds) Advanced Structured Materials, Vol. 30, Surface effects in solid mechanics - Models, Simulations and Applications. Springer-Verlag, Berlin, 2013, p. 105-121.