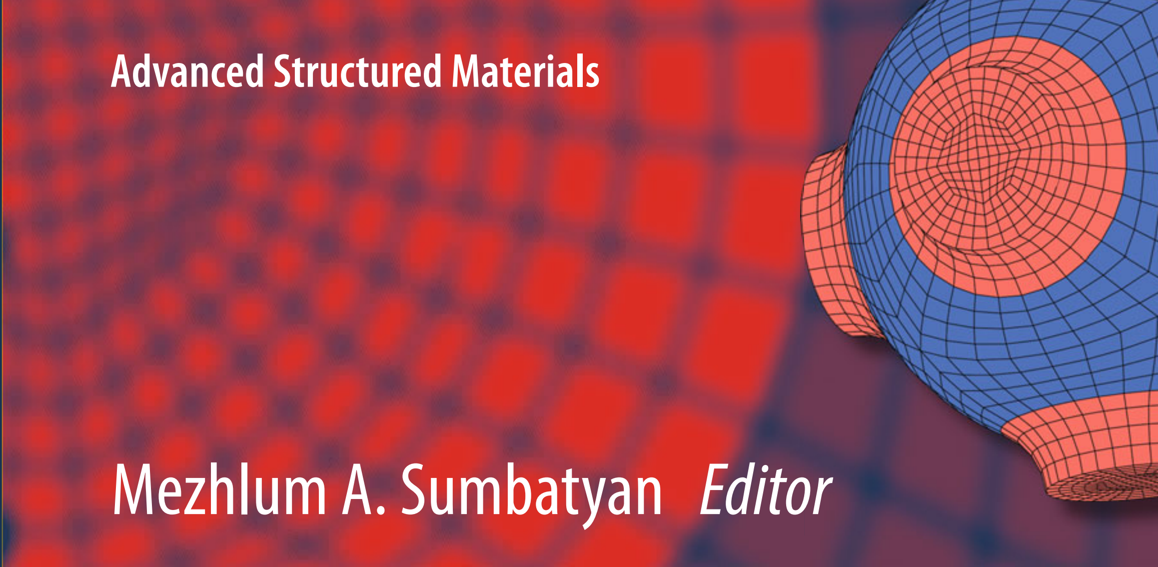
Advanced Structured Materials



Mezhlum A. Sumbatyan *Editor*

Wave Dynamics and Composite Mechanics for Microstructured Materials and Metamaterials

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Mezhlum A. Sumbatyan
Editor

Wave Dynamics and Composite Mechanics for Microstructured Materials and Metamaterials

Springer

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Foreword

In the last few years, the study of microstructured materials and metamaterials has become a trend in mechanics. Very often, trends and fashions are fading quickly not leaving deep traces in science.

This is not the case for the effort to design exotic materials, i.e., metamaterials whose mechanical behavior is tailored to meet specific functional requirements. They are indeed potentially of interest in applications where nonstandard mechanical, electromechanical, and acoustical properties, not exhibited by standard materials, are required. Their special behavior is governed by their microstructure, intending with this term their structure at a length scale much smaller (usually, smaller of at least one order of magnitude) than the wavelength of the macroscopic phenomenon they affect, rather than by their constituent materials.

The reader should be warned here: The topic is so important that many groups are working on it, by using different or sometimes very similar approaches. What is somehow puzzling is that the same subject, the same set of scientific and technological problems, and the same methodologies are sometimes labeled with different name (a detailed discussion of this point can be found in[1] or in[2]). Therefore, one finds works on architectured, advanced, multiscale, microstructured, complex, optimized (and so on) materials. Each label characterizes rather a group of researchers and not a really different research field.

In this foreword, and in this book, the preferred nomenclature uses the word "*metamaterial*" as it seems really suggestive: They are materials which go beyond as the Greek prefix "*meta*" exactly suggests this idea.

The interest of presented studies is increased by a circumstance which presented itself only recently: Indeed, the realization of metamaterials has become

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[1]F. dell'Isola, A. Della Corte, and I. Giorgio "Higher-gradient continua: The legacy of Piola, Mindlin, Sedov and Toupin and some future research perspectives." *Math. Mech. Solids* (2016): doi: 10.1177/1081286515616034.

[2]D. Del Vescovo and I. Giorgio "Dynamic problems for metamaterials: review of existing models and ideas for further research." *Int. J. Engng Sci* **80** (2014): 153–172.

economically viable by means of recent developments in some new manufacturing techniques such as 3D printing, roll-to-roll processing, electrospinning, photolithography and next-generation lithographies (extreme ultraviolet, X-ray, and charged-particle lithographies), dry etching, wet chemical etching, wet bulk micro-machining, thermal and mechanical energy-based removing, and micromolding.

Technology and theoretical disciplines do very often develop closely, one being a stimulus for the others. It is naive to believe that one can still theoretically design new products when disconnected from advanced manufacturing: For a good design, one needs to know the latest manufacturing processes and newest materials. In fact, changes of till-then established theoretical paradigms have been often, if not always, due to the advancement of new technology, which allows for new phenomenological evidence to arise. Given the availability of new technological possibilities as the ones mentioned before, nowadays, the main challenge in the field of metamaterials is the design of purpose-specific solutions to existing problems, for instance, in engineering and biomedical areas, by means of an intelligent exploitation of the properties of "ad hoc" architectured materials.

The desired outcome of the ongoing current research in the field of metamaterials is, therefore, not only the ability to predict the behavior of already existing materials (even with a possibly very complex behavior), but also assigned a certain (preferably exotic) desired behavior at the macroscale, the ability to prescribe constitutive and geometric characteristics at the microscale in order to get the selected macroscopic behavior.

Potential applications may include acoustically active materials, which behave like frequency filter and thus are able either to "cut" or to "pass" some frequency intervals, wind-excited structures, whose reliability can be, for instance, improved by means of targeted anisotropic behaviors and piezo- and flexo-electric induced vibration damping, and bone reconstructive surgery, because implants made of bioresorbable artificial materials guarantee a proper load-carrying capacity and a fast substitution of the device with newly formed bone.

It is well known that the functional adaptation process in bones is strongly related to the external load frequency. Therefore, dynamic properties of bone bioresorbable prostheses play a key role in the bone functional adaptation. For this reason, modal analyses are required to be performed in order to understand how dynamic features evolve with the remodeling process and are influenced by external mechanical factors.

In the design process, the mathematical modeling methodologies play a relevant role: in this book, this vision is clearly shown and exploited.

Mathematical modeling of materials has been developed in the nineteenth century on the basis of some assumptions, which are verified by the majority of natural materials and by standard materials used up to now in engineering. Usually, materials which show sophisticated and often unexpected behaviors are those whose microstructure is very complex, exhibits multiple characteristic length scales, involves coupled multiphysics phenomena, and shows strongly inhomogeneous physical properties at every characteristic length.

Clearly, that hypotheses assumed in classical physics for describing mechanical phenomena are not anymore suitable when one wants to model exotic artificial materials. The construction of the general theoretical framework for the description and prediction of the behavior of advanced architectured materials is the soundest ground for exploring those exotic phenomena.

Wave dynamics and mechanics of composite media with micro- and nanostructure, which might contain arrays of cracks, defects, and, eventually, micro- and nanosize elements coupling physical–mechanical fields of different nature, e.g., piezoelectric elements, are of crucial importance for the investigation of phenomena involved in this kind of materials. New theoretical advancements in these fields are needed to fully exploit the high potential of metamaterials and, in particular, fundamental methods, and models in the theory of wave problems and composite mechanics, which have already been proved to be powerful tools, need to be further developed. They will allow for the investigation of qualitative and quantitative properties exhibited by metamaterials: For instance, they will make possible the synthesis (i.e., the specification of the needed microstructure) when a desired behavior is required.

In conclusion, it is my sincerest hope that this volume enhances networking between some of the brightest scientists working in different fields, ranging from physics and applied mathematics to numerical analysis and materials science. Indeed, the published papers seem to me of the highest quality, as they show novel and relevant improvements of the specialistic literature.

Rome, Italy
October 2016

Francesco dell'Isola

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Mathematical Models and Finite Element Approaches for Nanosized Piezoelectric Bodies with Uncoulped and Coupled Surface Effects

Victor A. Eremeyev and A.V. Nasedkin

Abstract In this chapter the dynamic problems for piezoelectric nanosized bodies with account for coupled damping and surface effects are considered. For these problems we propose new mathematical model which generalizes the models of the elastic medium with damping in sense of the Rayleigh approach and with surface effects for the cases of piezoelectric materials. Our model of attenuation and surface effects has coupling properties between mechanical and electric fields, both for the damping terms and constitutive equations for piezoelectric materials on the surface. For solving the problems stated the finite element approximations are discussed. A set of effective finite element schemes is examined for finding numerical solutions of week statements for nonstationary problems, steady-state oscillation problems, modal problems and static problems within the framework of modelling of piezoelectric nanosized materials with damping and surface effects. For transient and harmonic problems, we demonstrate that the proposed models allow the use of the mode superposition method. In addition, we note that for transient and static problems we can use efficient finite element algorithms for solving the systems of linear algebraic equations with symmetric quasi-definite matrices both in the case of uncoupled surface effects and in the case of coupled surface effects.

Keywords Surface elasticity · Piezoelectricity · Finite element method · Rayleigh damping

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1 Introduction

The most popular model of the surface elasticity [20, 32, 34] is the Gurtin-Murdoch model [19] which used in nanomechanics, see [8, 9, 38]. The Gurtin–Murdoch model was extended by Steigmann and Ogden [35, 36]. The mentioned models consider elastic media whereas the extension for piezoelectric and magnetoelastic media was introduced in [21, 39]. The existence of surface stresses leads to changes in behaviour of stresses and deformations in the vicinity of stress concentrators, such as crack tips, see [22–24]. In the media with surface stresses new type of waves is possible, that are anti-plane (shear) surface waves [13, 14] which absent in classic elasticity. The mathematical study of boundary-value problems in the elasticity with surface stresses where performed in [1, 2, 10, 11, 33] where existence and uniqueness of weak and strong solutions were proved. Existence and uniqueness of weak solutions for modal problem considering surface effects in solids with coupling of deformations and electric field was proved in [12, 27].

In the one of the first papers in the field of piezoelectricity with surface effects [21] it was proposed new model of a nanosized piezoelectric solid with introduction into the functional of energy surface integrals depending on the surface stresses and strains. Here the surface dielectric permittivities and the surface piezomoduli are introduced as additional material parameters. For the static axially symmetric problem for a piezoelectric ring with thin electrodes at its faces, the surface effects are taken into account in the boundary conditions for stresses. From the mechanical point of view the main idea of [21] consists of introduction of a piezoelectric film at the surface of an nanosized piezoelectric solid. The constitutive equations of the film determine the relation between the surface stresses and the surface electric displacement vector with the strains and the electrical field including its component normal to surface.

Similar approach was applied in analysis of piezoelectric nanowires, beams, and plates in [37, 44–49, 53], of a plate oscillations in [51, 52, 54]. Propagation of the Bleustein–Gulyaev waves in a piezoelectric half-space with thin surface piezoelectric layer are studied in [6] with asymptotic expansions technique. Using atomistic models and multiscale analysis in [31] the mechanical and electrostatic stresses of Piola–Kirchhoff-type are reconstructed. Formulae for the effective shear modulus of a fiber reinforced piezoelectric composite was obtained in [42] using a self-consistent method. Investigations of effective moduli for nanoisized piezoelectric composites were continued in [5, 15, 25, 41, 43] and etc.

Magnetoelectric nanosized composites were analysed in [17, 28, 29, 40] and etc.

Theoretical investigations of piezoelectric and magnetoelectric nanosized materials with surface effects and imperfect interface models were presented in [7, 12, 16–18, 30]. Note that dynamic models for piezoelectric and magnetoelectric nanosized bodies with damping and surface effects were suggested only in [27–29], but for uncoupled dependencies between mechanical and electric or magnetoelectric surface fields.

The main goal of our investigation is to present the mathematical study of the dynamic boundary-value problems for pizoelectric solids with damping and coupling between surface mechanical and electric fields. In this paper we propose the new models for nanosized piezoelectric bodies with surface effects in development of corresponding investigations of nanosized active materials earlier presented in [27–29]. Here we formulate the system of differential equations with damping properties, the special boundary conditions with taking into account the coupled surface effects, damping and the initial conditions for piezoelectric nanosized bodies.

For numerical solution of the dynamic problems with damping and surface effects we propose the finite element approximations and the corresponding generalized matrix problems. We note that the standard finite element software could be used with additional introduction of surface piezoelectric elements with structural membrane option. We demonstrate that the finite element systems for coupled problems for piezoelectric nanosized bodies can be represented in the form of a system of linear algebraic equations with symmetric saddle point quasi-definite matrices. We also describe special efficient approaches to solve the resulting finite element equations for transient, harmonic, modal and static problems.

2 Model of Piezoelectric Materials with Damping and Surface Effects

Let $\Omega \in \mathrm{R}^3$ be a region occupied by a piezoelectric material; $\Gamma = \partial\Omega$ is the boundary of this region; $\mathbf{n}$ is the vector of the external unit normal to Γ; $\mathbf{x} = \{x_1, x_2, x_3\}$ is the vector of the special coordinates; t is the time; $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ is the vector of mechanical displacements; $\varphi = \varphi(\mathbf{x}, t)$ is the scalar function of electric potential. The system of differential equations for piezoelectric body with damping effects in the volume Ω can be present in the form

$$\nabla \cdot \boldsymbol{\sigma} + \rho\,\mathbf{f} = \rho\,(\ddot{\mathbf{u}} + \alpha_d \dot{\mathbf{u}}), \quad \nabla \cdot \mathbf{D} = q_\Omega, \tag{1}$$

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

$$\mathbf{D} + \zeta_d \dot{\mathbf{D}} = \mathbf{e} : (\boldsymbol{\varepsilon} + \zeta_d \dot{\boldsymbol{\varepsilon}}) + \boldsymbol{\kappa} \cdot \mathbf{E}, \tag{3}$$

$$\boldsymbol{\varepsilon} = (\nabla\mathbf{u} + (\nabla\mathbf{u})^*)/2, \quad \mathbf{E} = -\nabla\varphi, \tag{4}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are the second-order stress and strain tensors; $\mathbf{D}$ and $\mathbf{E}$ are the electric flux density vector or the electric displacement vector and the electric field vector; ρ is the mass density of the material; $\mathbf{c} = \mathbf{c}^E$ is the fourth-order tensor of elastic stiffness moduli; $\mathbf{e}$ is the third-order tensor of piezoelectric moduli; $\boldsymbol{\kappa} = \boldsymbol{\kappa}^S = \boldsymbol{\varepsilon}^S$ is the second-order tensor of dielectric permittivity moduli; α_d, β_d, ζ_d are the damping coefficients; $\mathbf{f}$ is the vector of mass forces; q_Ω is the density of free electric charges (usually, $q_\Omega = 0$); $\dot{\mathbf{u}} = \partial\mathbf{u}/\partial t$; $\ddot{\mathbf{u}} = \partial^2\mathbf{u}/\partial^2 t$; $(\ldots)^T$ is the transpose operation; $(\ldots):(\ldots)$ is the double scalar product operation.

We suppose that the material moduli have the usual symmetry properties: $c_{ijkl} = c_{jikl} = c_{klij}$, $e_{ikl} = e_{ilk}$, $\kappa_{kl} = \kappa_{lk}$. In addition to this for the positive definiteness of the intrinsic energy for the piezoelectric medium the following inequalities must be satisfied ($\forall\ \boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^T, \mathbf{E}$), $\exists\, W_\Omega > 0$:

$$\boldsymbol{\varepsilon}^T : \mathbf{c} : \boldsymbol{\varepsilon} + \mathbf{E}^T \cdot \boldsymbol{\kappa} \cdot \mathbf{E} \geq W_\Omega(\boldsymbol{\varepsilon}^T : \boldsymbol{\varepsilon} + \mathbf{E}^T \cdot \mathbf{E}).$$

In models (1)–(4) for the piezoelectric material, we use a generalized Rayleigh method of damping evaluation [3, 26, 28, 29], which is admissible for many practical applications. When $\zeta_d = 0$ in Eq. (3), we have the model for taking into account of mechanical damping in piezoelectric media which is adopted in the case of elastic and piezoelectric materials in several well-known finite element packages. More complicated model (1)–(4) extends the Kelvin's model to the case of piezoelectric media. It has been shown that the model (2) and (3) with $\beta_d = \zeta_d$ satisfies the conditions of the energy dissipation and has the possibility of splitting the finite element system into independent equations for the separate modes in the case of piezoelectric media, see also Sect. 4.

For nanosized piezoelectric body we assume that on its boundary Γ the surface stress and surface electric flux exist. For these quantities we accept the Gurtin–Murdoch model:

$$\mathbf{n} \cdot \boldsymbol{\sigma} = \nabla^s \cdot \boldsymbol{\sigma}^s + \mathbf{p}, \qquad \mathbf{x} \in \Gamma, \tag{5}$$

$$\mathbf{n} \cdot \mathbf{D} = \nabla^s \cdot \mathbf{D}^s - q, \qquad \mathbf{x} \in \Gamma, \tag{6}$$

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 $\mathbf{n}$ to Γ_σ; $\boldsymbol{\sigma}^s$ is the second-order tensor of surface stress; $\mathbf{D}^s$ is the surface electric flux density vector; $\mathbf{p}$ is the vector of mechanical stress; q is the surface density of electric charge.

Here, $\mathbf{p}$ and q are the known (active) or unknown (reactive) surface quantities according to the boundary conditions.

For surface stress $\boldsymbol{\sigma}^s$ and surface electric flux $\mathbf{D}^s$ in general case we take the coupled constitutive relations

$$\boldsymbol{\sigma}^s = \mathbf{c}^s : (\boldsymbol{\varepsilon}^s + \beta_d \dot{\boldsymbol{\varepsilon}}^s) - \mathbf{e}^{sT} \cdot \mathbf{E}^s, \tag{7}$$

$$\mathbf{D}^s + \zeta_d \dot{\mathbf{D}}^s = \mathbf{e}^s : (\boldsymbol{\varepsilon}^s + \zeta_d \dot{\boldsymbol{\varepsilon}}^s) + \boldsymbol{\kappa}^s \cdot \mathbf{E}^s, \tag{8}$$

where

$$\boldsymbol{\varepsilon}^s = (\nabla^s \mathbf{u}^s + (\nabla^s \mathbf{u}^s)^T)/2, \quad \mathbf{u}^s = \mathbf{A} \cdot \mathbf{u}, \quad \mathbf{A} = \mathbf{I} - \mathbf{n} \otimes \mathbf{n}, \quad \mathbf{E}^s = -\nabla^s \varphi, \tag{9}$$

$\mathbf{I}$ is the identity matrix; $\mathbf{c}^s$, $\mathbf{e}^s$, $\boldsymbol{\kappa}^s$ are the surface tensors of elastic stiffness moduli, piezoelectric moduli and dielectric permittivity moduli, respectively.

We suppose that the tensors of surface material moduli have the similar properties that the tensors of volume material moduli, but relatively to surface strains $\boldsymbol{\varepsilon}^s$ and surface electric field vector $\mathbf{E}^s$, i.e. $c^s_{ijkl} = c^s_{jikl} = c^s_{klij}, e^s_{ikl} = e^s_{ilk}, \kappa^s_{kl} = \kappa^s_{lk}$, and surface energy is positive definiteness ($\forall\ \boldsymbol{\varepsilon}^s = \boldsymbol{\varepsilon}^{sT}, \mathbf{E}^s$), $\exists\, W_\Gamma > 0$:

$$\boldsymbol{\varepsilon}^{sT} : \mathbf{c}^s : \boldsymbol{\varepsilon}^s + \mathbf{E}^{sT} \cdot \boldsymbol{\kappa}^s \cdot \mathbf{E}^s \geq W_\Gamma(\boldsymbol{\varepsilon}^{sT} : \boldsymbol{\varepsilon}^s + \mathbf{E}^{sT} \cdot \mathbf{E}^s).$$

The boundary and the initial conditions should be added to the system of equations (1)–(9). The boundary conditions are mechanical and electric types.

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 $\boldsymbol{\sigma}^s$ and the vector of mechanical stress $\mathbf{p}_\Gamma$, i.e.

$$\mathbf{p} = \mathbf{p}_\Gamma, \qquad \mathbf{x} \in \Gamma_\sigma, \tag{10}$$

and so, in accordance with (5)

$$\mathbf{n} \cdot \boldsymbol{\sigma} = \nabla^s \cdot \boldsymbol{\sigma}^s + \mathbf{p}_\Gamma, \qquad \mathbf{x} \in \Gamma_\sigma. \tag{11}$$

On the part Γ_u we pose known the mechanical displacements vector $\mathbf{u}_\Gamma$

$$\mathbf{u} = \mathbf{u}_\Gamma, \qquad \mathbf{x} \in \Gamma_u, \tag{12}$$

and so, in (6) $\mathbf{p}$ is unknown reactive surface load vector on Γ_u.

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 we pose known the surface density of electric charge q_Γ

$$q = q_\Gamma, \qquad \mathbf{x} \in \Gamma_D, \tag{13}$$

i.e. in accordance with (6) on Γ_D hold the following conditions

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

and usually, $q_\Gamma = 0$.

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

$$\varphi = \Phi_j, \quad \mathbf{x} \in \Gamma_{\varphi j}, \quad j \in J_Q, \tag{15}$$

$$\int_{\Gamma_{\varphi j}} q\, d\Gamma = Q_j, \quad I_j = \pm \dot{Q}_j, \qquad \mathbf{x} \in \Gamma_{\varphi j}, \quad j \in J_Q, \tag{16}$$

$$\varphi = V_j, \qquad \mathbf{x} \in \Gamma_{\varphi j}, \quad j \in J_V, \quad \Gamma_{j0} \neq \emptyset, \tag{17}$$

where the variables $\boldsymbol{\Phi}_j$, V_j do not depend on $\mathbf{x}$; Q_j is the overall electric charge on $\Gamma_{\varphi j}$, the sign "±" in (16) is chosen in accordance with the accepted direction of the current I_j in the electric circuit, and by using (6) we can rewrite the relation (16) in the other form

$$\int_{\Gamma_{\varphi j}} \mathbf{n} \cdot \mathbf{D}\, d\Gamma - \int_{\Gamma_{\varphi j}} \nabla^s \cdot \mathbf{D}^s\, d\Gamma = -Q_j, \quad I_j = \pm \dot{Q}_j, \qquad \mathbf{x} \in \Gamma_{\varphi j}, \quad j \in J_Q. \tag{18}$$

For transient problems it is also necessary to pose initial conditions, which can be written as

$$\mathbf{u} = \mathbf{u}_*(\mathbf{x}), \quad \dot{\mathbf{u}} = \mathbf{r}_*(\mathbf{x}), \quad t = 0, \quad \mathbf{x} \in \Omega, \tag{19}$$

where $\mathbf{u}_*(\mathbf{x})$ and $\mathbf{r}_*(\mathbf{x})$ are the known initial values of the corresponding fields.

Formulas (1)–(19) represent the statement of the transient problem for piezoelectric body with the generalized Rayleigh damping and with account for coupled surface effects for mechanical and electric fields.

If in (7) and (8) we assume $\mathbf{e}^s = 0$, i.e. surface piezomoduli are equal to zero, then we obtain the uncoupled constitutive equations, when the mechanical surface stress $\boldsymbol{\sigma}^s$ depend only on the surface strain $\boldsymbol{\varepsilon}^s$, and surface electric flux $\mathbf{D}^s$ depend only on the surface electric field vector $\mathbf{E}^s$. This more simple model we are investigated for different dynamic problems earlier in [12, 27–29].

3 Week Formulations of Dynamic Problem

In order to formulate the weak or generalized statement of dynamic transient problem for nanosized piezoelectric solid we scalar multiply Eq. (1) by some sufficiently differentiable vector-function $\mathbf{v}$ and functions χ, which satisfies following principal boundary conditions, i.e.

$$\mathbf{v} = 0, \qquad \mathbf{x} \in \Gamma_u, \tag{20}$$

$$\chi = X_j, \quad \mathbf{x} \in \Gamma_{\varphi j}, \quad j \in J_Q, \tag{21}$$

$$\chi = 0, \qquad \mathbf{x} \in \Gamma_{\varphi j}, \quad j \in J_V, \tag{22}$$

where X_j are the arbitrary constant values on $\Gamma_{\varphi j} \subset \Gamma_Q$.

By integrating the obtained equations over Ω and by using the standard technique of the integration by parts with Eqs. (2)–(18) and (20)–(22), we obtain

$$\rho(\mathbf{v}, \ddot{\mathbf{u}}) + d(\mathbf{v}, \dot{\mathbf{u}}) + c(\mathbf{v}, \mathbf{u}) + e_u(\varphi, \mathbf{v}) = \tilde{L}_u(\mathbf{v}), \tag{23}$$

$$-\,e_{\varphi}(\chi, \mathbf{u} + \zeta_d \dot{\mathbf{u}}) + \kappa(\chi, \varphi) = \tilde{L}_{\varphi}(\chi) + \zeta_d \frac{\partial}{\partial t} \tilde{L}_{\varphi}(\chi), \tag{24}$$

where

$$\rho(\mathbf{v}, \mathbf{u}) = \int_{\Omega} \rho \mathbf{v}^T \cdot \mathbf{u} \, d\Omega, \quad d(\mathbf{v}, \mathbf{u}) = \alpha_d \rho(\mathbf{v}, \mathbf{u}) + \beta_d c(\mathbf{v}, \mathbf{u}), \tag{25}$$

$$c(\mathbf{v}, \mathbf{u}) = c_{\Omega}(\mathbf{v}, \mathbf{u}) + c_{\Gamma}(\mathbf{v}, \mathbf{u}), \quad \kappa(\chi, \varphi) = \kappa_{\Omega}(\chi, \varphi) + \kappa_{\Gamma}(\chi, \varphi), \tag{26}$$

$$e_u(\varphi, \mathbf{v}) = e_{\Omega}(\varphi, \mathbf{v}) + e_{\Gamma\sigma}(\varphi, \mathbf{v}), \quad e_{\varphi}(\chi, \mathbf{u}) = e_{\Omega}(\chi, \mathbf{u}) + e_{\Gamma D}(\chi, \mathbf{u}), \tag{27}$$

$$c_{\Omega}(\mathbf{v}, \mathbf{u}) = \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{v}) : \mathbf{c} : \boldsymbol{\varepsilon}(\mathbf{u}) \, d\Omega, \quad c_{\Gamma}(\mathbf{v}, \mathbf{u}) = \int_{\Gamma_\sigma} \boldsymbol{\varepsilon}^s(\mathbf{v}) : \mathbf{c}^s : \boldsymbol{\varepsilon}^s(\mathbf{u}) \, d\Gamma, \tag{28}$$

$$\kappa_{\Omega}(\chi, \varphi) = \int_{\Omega} \mathbf{E}(\chi) \cdot \boldsymbol{\kappa} \cdot \mathbf{E}(\varphi) \, d\Omega, \quad \kappa_{\Gamma}(\chi, \varphi) = \int_{\Gamma_D} \mathbf{E}^s(\chi) \cdot \boldsymbol{\kappa}^s \cdot \mathbf{E}^s(\varphi) \, d\Gamma, \tag{29}$$

$$e_{\Omega}(\varphi, \mathbf{v}) = -\int_{\Omega} \mathbf{E}(\varphi) \cdot \mathbf{e} : \boldsymbol{\varepsilon}(\mathbf{v}) \, d\Omega, \;\; e_{\Gamma\sigma}(\varphi, \mathbf{v}) = -\int_{\Gamma_\sigma} \mathbf{E}^s(\varphi) \cdot \mathbf{e}^s : \boldsymbol{\varepsilon}^s(\mathbf{v}) \, d\Gamma, \tag{30}$$

$$e_{\Gamma D}(\chi, \mathbf{u}) = -\int_{\Gamma_D} \mathbf{E}^s(\chi) \cdot \mathbf{e}^s : \boldsymbol{\varepsilon}^s(\mathbf{u}) \, d\Gamma, \tag{31}$$

$$\tilde{L}_u(\mathbf{v}) = \int_{\Omega} \mathbf{v} \cdot \rho \mathbf{f} \, d\Omega + \int_{\Gamma_\sigma} \mathbf{v} \cdot \mathbf{p}_{\Gamma} \, d\Gamma, \tag{32}$$

$$\tilde{L}_{\varphi}(\chi) = \int_{\Omega} \chi q_{\Omega} \, d\Omega + \int_{\Gamma_D} \chi q_{\Gamma} + \sum_{k \in J_Q} X_k Q_k \, d\Gamma. \tag{33}$$

The weak form of the initial conditions (19) can be represent by the relations

$$\rho(\mathbf{v}, \mathbf{u}) = \rho(\mathbf{v}, \mathbf{u}_*), \quad \rho(\mathbf{v}, \dot{\mathbf{u}}) = \rho(\mathbf{v}, \mathbf{r}_*), \quad t = 0. \tag{34}$$

Further we present the functions $\mathbf{u}$ and φ as

$$\mathbf{u} = \mathbf{u}_0 + \mathbf{u}_b, \quad \varphi = \varphi_0 + \varphi_b, \tag{35}$$

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

$$\mathbf{u}_0 = 0, \quad \mathbf{u}_b = \mathbf{u}_{\Gamma}, \qquad \mathbf{x} \in \Gamma_u, \tag{36}$$

$$\varphi_0 = \boldsymbol{\Phi}_{0j}, \quad \varphi_b = \boldsymbol{\Phi}_{bj}, \quad \boldsymbol{\Phi}_j = \boldsymbol{\Phi}_{0j} + \boldsymbol{\Phi}_{bj}, \quad \mathbf{x} \in \Gamma_{\varphi j}, \quad j \in J_Q, \tag{37}$$

$$\varphi_0 = 0, \quad \varphi_b = V_j, \qquad \mathbf{x} \in \Gamma_{\varphi j}, \quad j \in J_V. \tag{38}$$

Using (35), we can modify the system (23) and (24) into the form

$$\rho(\mathbf{v}, \ddot{\mathbf{u}}_0) + d(\mathbf{v}, \dot{\mathbf{u}}_0) + c(\mathbf{v}, \mathbf{u}_0) + e_u(\varphi_0, \mathbf{v}) = L_u(\mathbf{v}), \tag{39}$$

$$-e_\varphi(\chi, \mathbf{u}_0 + \zeta_d \dot{\mathbf{u}}_0) + \kappa(\chi, \varphi_0) = L_\varphi(\chi), \tag{40}$$

where

$$L_u(\mathbf{v}) = \tilde{L}_u(\mathbf{v}) - \rho(\mathbf{v}, \ddot{\mathbf{u}}_b) - d(\mathbf{v}, \dot{\mathbf{u}}_b) - c(\mathbf{v}, \mathbf{u}_b) - e_u(\varphi_b, \mathbf{v}), \tag{41}$$

$$L_\varphi(\chi) = \tilde{L}_\varphi(\chi) + \zeta_d \frac{\partial}{\partial t} \tilde{L}_\varphi(\chi) + e_\varphi(\chi, \mathbf{u}_b + \zeta_d \dot{\mathbf{u}}_b) - \kappa(\chi, \varphi_b). \tag{42}$$

We denote with the Hilbert vector space H_u the closure of the set of vector functions $\mathbf{v} \in \mathrm{C}^1$, satisfying homogeneous principal boundary condition (20), with the norm generated by bilinear form defined in the first relation (26) and in (28).

We also denote with the Hilbert space H_φ the closure of the set of function $\varphi \in C^1$, satisfying boundary condition (21) and (22), in the norm generated by scalar production from the second relation (26) and (29).

Finally, we introduce the functional spaces $Q_u = L^2(0, T; H_u)$ and $Q_\varphi = L^2(0, T; H_\varphi)$, where for Banach space X with norm $||.||_X$ the space $L^2(0, T; X)$ is the space of class functions $t \to f(t)$ from $[0, T]$ into X which satisfy the condition

$$||f||^2_{L^2(0,T;X)} = \int_0^T ||f||^2_X \, dt < \infty.$$

Now we can define generalized or weak solution of dynamic problem (1)–(19) using these functional spaces.

Definition. The functions $\mathbf{u} = \mathbf{u}_0 + \mathbf{u}_b$, $\mathbf{u}_0 \in Q_u$; $\varphi = \varphi_0 + \varphi_b$, $\varphi_0 \in Q_\varphi$ are the weak solution of dynamic problem for the piezoelectric body with damping and coupled surface effects, if Eqs. (39) and (40) with (25)–(33), (41) and (42) are satisfied for $\forall t \in [0, T]$; $\mathbf{v} \in H_u$, $\chi \in H_\varphi$, and the initial conditions (34) are also hold.

It is important to mark that after transfer Eqs. (23) and (24) to (39) and (40), we obtain

$$e_{\Gamma\sigma}(\varphi_0, \mathbf{v}) = e_{\Gamma\sigma D}(\varphi_0, \mathbf{v}) = -\int_{\Gamma_{\sigma D}} \mathbf{E}^s(\varphi_0) \cdot \mathbf{e}^s : \boldsymbol{\varepsilon}^s(\mathbf{v}) \, d\Gamma, \tag{43}$$

$$e_{\Gamma D}(\chi, \mathbf{u}_0) = e_{\Gamma\sigma D}(\chi, \mathbf{u}_0) = -\int_{\Gamma_{\sigma D}} \mathbf{E}^s(\chi) \cdot \mathbf{e}^s : \boldsymbol{\varepsilon}^s(\mathbf{u}_0) \, d\Gamma, \tag{44}$$

where $\Gamma_{\sigma D} = \Gamma_\sigma \cap \Gamma_D$, as far as $\mathbf{E}^s(\varphi_0) = 0$ for $\mathbf{x} \in \Gamma_\sigma \setminus \Gamma_{\sigma D}$, and $\boldsymbol{\varepsilon}^s(\mathbf{u}_0) = 0$ for $\mathbf{x} \in \Gamma_D \setminus \Gamma_{\sigma D}$.

These equations allow us to obtain later the symmetric systems, because from (43) and (44) with (27), (30) and (31) it is follow that

$$e_u(\varphi_0, \mathbf{v}) = e_\varphi(\varphi_0, \mathbf{v}), \quad e_\varphi(\chi, \mathbf{u}_0) = e_u(\chi, \mathbf{u}_0).$$

4 Finite Element Approaches

4.1 Nonstationary Problems

For numerical solving the problems (34), (39) and (40) we will use the finite element method. Let Ω_h be the region of the corresponding finite element mesh: $\Omega_h \subset \Omega$, $\Omega_h = \cup_k \Omega_{ek}$, where Ω_{ek} is a separate volume or surface finite element with number k. On this mesh we shall find the approximation to the weak solution $\{\mathbf{u}_{0h} \approx \mathbf{u}_0$, $\varphi_{0h} \approx \varphi_0\}$ in the form

$$\mathbf{u}_h(\mathbf{x}, t) = \mathbf{N}_u^T(\mathbf{x}) \cdot \mathbf{U}(t), \quad \varphi_h(\mathbf{x}, t) = \mathbf{N}_\varphi^T(\mathbf{x}) \cdot \boldsymbol{\Phi}(t), \tag{45}$$

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

We represent the projecting functions $\mathbf{v}$ and χ in finite-dimensional spaces by the formulae

$$\mathbf{v}^T = \delta\mathbf{U}^T \cdot \mathbf{N}_u(\mathbf{x}), \quad \chi = \mathbf{N}_\varphi^T \cdot \delta\boldsymbol{\Phi} = \delta\boldsymbol{\Phi}^T \cdot \mathbf{N}_\varphi, \tag{46}$$

Note that we can use the same nodal degrees of freedom and the shape functions for volume and surface elements, or rather, in accordance with (9) we will consider the surface shape functions for displacements as a reduction of volume shape function on the surface elements by formula $\mathbf{N}_u^{sT} = \mathbf{A} \cdot \mathbf{N}_u^T$, and $\mathbf{N}_\varphi^s = \mathbf{N}_\varphi$.

Substituting (45) and (46) into the problem (39) and (40) with (25)–(33), (41) and (42) for Ω_h, $\Gamma_h = \partial\Omega_h$, $\Gamma_{\sigma h}$, Γ_{Dh}, $\Gamma_{\sigma Dh}$, we obtain the finite element system of ordinary differential equations with respect to time

$$\mathbf{M}_{uu} \cdot \ddot{\mathbf{U}} + \mathbf{C}_{uu} \cdot \dot{\mathbf{U}} + \mathbf{K}_{uu} \cdot \mathbf{U} + \mathbf{K}_{u\varphi} \cdot \boldsymbol{\Phi} = \mathbf{F}_u, \tag{47}$$

$$-\mathbf{K}_{u\varphi}^* \cdot (\mathbf{U} + \zeta_d \dot{\mathbf{U}}) + \mathbf{K}_{\varphi\varphi} \cdot \boldsymbol{\Phi} = \mathbf{F}_\varphi, \tag{48}$$

with the initial conditions

$$\mathbf{U}(0) = \mathbf{U}_*, \quad \dot{\mathbf{U}}(0) = \mathbf{R}_*, \tag{49}$$

which are derived from the corresponding initial conditions (19) or (34).

Here,

$$\mathbf{M}_{uu} = \int_{\Omega_h} \rho \mathbf{N}_u \cdot \mathbf{N}_u^T \, d\Omega, \quad \mathbf{C}_{uu} = \alpha_d \mathbf{M}_{uu} + \beta_d \mathbf{K}_{uu}, \tag{50}$$

$$\mathbf{K}_{uu} = \mathbf{K}_{\Omega uu} + \mathbf{K}_{\Gamma uu}, \quad \mathbf{K}_{u\varphi} = \mathbf{K}_{\Omega u\varphi} + \mathbf{K}_{\Gamma u\varphi}, \quad \mathbf{K}_{\varphi\varphi} = \mathbf{K}_{\Omega\varphi\varphi} + \mathbf{K}_{\Gamma\varphi\varphi}, \tag{51}$$

$$\mathbf{K}_{\Omega uu} = \int_{\Omega_h} \mathbf{B}_u^T \cdot \mathbf{c} \cdot \mathbf{B}_u \, d\Omega, \quad \mathbf{K}_{\Gamma uu} = \int_{\Gamma_{\sigma h}} \mathbf{B}_u^{sT} \cdot \mathbf{c}^s \cdot \mathbf{B}_u^s \, d\Gamma, \tag{52}$$

$$\mathbf{K}_{\Omega u\varphi} = \int_{\Omega_h} \mathbf{B}_u^T \cdot \mathbf{e}^T \cdot \mathbf{B}_\varphi \, d\Omega, \quad \mathbf{K}_{\Gamma u\varphi} = \int_{\Gamma_{\sigma Dh}} \mathbf{B}_u^{sT} \cdot \mathbf{e}^{sT} \cdot \mathbf{B}_\varphi^s \, d\Gamma, \tag{53}$$

$$\mathbf{K}_{\Omega\varphi\varphi} = \int_{\Omega_h} \mathbf{B}_\varphi^T \cdot \boldsymbol{\kappa} \cdot \mathbf{B}_\varphi \, d\Omega, \quad \mathbf{K}_{\Gamma\varphi\varphi} = \int_{\Gamma_{Dh}} \mathbf{B}_\varphi^{sT} \cdot \boldsymbol{\kappa}^s \cdot \mathbf{B}_\varphi^s \, d\Gamma, \tag{54}$$

$$\mathbf{B}_u^{(s)} = \mathbf{L}(\nabla^{(s)}) \cdot \mathbf{N}_u^{(s)T}, \;\; \mathbf{B}_\varphi^{(s)} = \nabla \mathbf{N}_\varphi^{(s)T}, \;\; \mathbf{L}^T(\nabla^{(s)}) = \begin{bmatrix} \partial_1^{(s)} & 0 & 0 & 0 & \partial_3^{(s)} & \partial_2^{(s)} \\ 0 & \partial_2^{(s)} & 0 & \partial_3^{(s)} & 0 & \partial_1^{(s)} \\ 0 & 0 & \partial_3^{(s)} & \partial_2^{(s)} & \partial_1^{(s)} & 0 \end{bmatrix}. \tag{55}$$

The vectors $\mathbf{F}_u$, $\mathbf{F}_\varphi$ in (47) and (48) are obtained from the corresponding right parts of the weak statements (39) and (40) with (25)–(33), (41) and (42) and the finite element representations (46).

In (52)–(54) we use vector-matrix forms for the moduli [4]: $\mathbf{c}^{(s)}$ is the 6×6 matrix of elastic moduli, $c_{\alpha\beta}^{(s)} = c_{ijkl}^{(s)}$; $\alpha, \beta = 1, \ldots, 6$; $i, j, k, l = 1, 2, 3$ with the correspondence law $\alpha \leftrightarrow (ij)$, $\beta \leftrightarrow (kl)$, $1 \leftrightarrow (11)$, $2 \leftrightarrow (22)$, $3 \leftrightarrow (33)$, $4 \leftrightarrow (23) = (32)$, $5 \leftrightarrow (13) = (31)$, $6 \leftrightarrow (12) = (21)$; $\mathbf{e}^{(s)}$ is the 3×6 matrix of piezoelectric moduli ($e_{i\beta}^{(s)} = e_{ikl}^{(s)}$).

We note that in (50)–(54) the matrices of mass and stiffness $\mathbf{M}_{uu}$, $\mathbf{K}_{\Omega uu}$, and nodal mechanical force vector $\mathbf{F}_u$ are formed in the same way as for purely elastic body, and the matrices $\mathbf{K}_{\Omega u\varphi}$, $\mathbf{K}_{\Omega\varphi\varphi}$ and nodal electric force vector $\mathbf{F}_\varphi$ are identical to the corresponding matrices and vector for piezoelectric bodies. The matrices $\mathbf{K}_{\Gamma uu}$, $\mathbf{K}_{\Gamma u\varphi}$ and $\mathbf{K}_{\Gamma\varphi\varphi}$ are defined by the surface mechanical, piezoelectric and dielectric effects. The matrix $\mathbf{K}_{\Gamma uu}$ is analogous to the stiffness matrix for surface elastic membranes and the matrix $\mathbf{K}_{\Gamma\varphi\varphi}$ is the matrix 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 piezoelectric elements with structural membrane option along with ordinary solid piezoelectric finite elements.

4.2 Static Problems

In the case of static problems all dependencies on time t are absent, and the finite element system (47) and (48) reduces to the form

$$\mathbf{K} \cdot \mathbf{a} = \mathbf{F}, \tag{56}$$

where

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{u\varphi} \\ \mathbf{K}_{u\varphi}^T & -\mathbf{K}_{\varphi\varphi} \end{bmatrix}, \quad \mathbf{a} = \begin{bmatrix} \mathbf{U} \\ \boldsymbol{\Phi} \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} \mathbf{F}_u \\ -\mathbf{F}_\varphi \end{bmatrix}. \tag{57}$$

The matrix **K** in (56) and (57) is symmetric and quasi-definite. Thus, problem (56) possesses the main calculating properties of finite element matrices for the theory of piezoelectricity, and therefore it can be solved by the same effective algorithms as the analogous problems for ordinary piezoelectric media. For example, we can use the set of algorithms for finite element analysis with symmetric and quasi-definite matrices represented in ACELAN package [26, 29]: the degree of freedom rotations, boundary condition settings, LDL^T-factorization or Cholesky method for solving the system of linear algebraic equations, and others.

4.3 Steady-State Oscillation Problems

When all external loads and degree of freedom constraints vary with the same harmonic law $\exp[j\omega t]$, i.e. $\mathbf{F}_u = \tilde{\mathbf{F}}_u \exp[j\omega t]$, $\mathbf{F}_\varphi = \tilde{\mathbf{F}}_\varphi \exp[j\omega t]$, we have the behavior of steady-state or harmonic oscillations ($\mathbf{a} = \tilde{\mathbf{a}} \exp[j\omega t]$, $\mathbf{U} = \tilde{\mathbf{U}} \exp[j\omega t]$, $\boldsymbol{\Phi} = \tilde{\boldsymbol{\Phi}} \exp[j\omega t]$). In this case, as it is obvious from (47) and (48), we have a system of linear algebraic equations (56) for the amplitude values $\tilde{\mathbf{a}}$ with

$$\mathbf{K} = \begin{bmatrix} -\omega^2\mathbf{M}_{uu} + j\omega\mathbf{C}_{uu} + \mathbf{K}_{uu} & \mathbf{K}_{u\varphi} \\ \mathbf{K}_{u\varphi}^T & -\mu\mathbf{K}_{\varphi\varphi} \end{bmatrix}, \quad \tilde{\mathbf{a}} = \begin{bmatrix} \tilde{\mathbf{U}} \\ \tilde{\boldsymbol{\Phi}} \end{bmatrix}, \quad \tilde{\mathbf{F}} = \begin{bmatrix} \tilde{\mathbf{F}}_u \\ -\mu\tilde{\mathbf{F}}_\varphi \end{bmatrix}, \tag{58}$$

where $\mu = (1 + j\omega\zeta_d)^{-1}$.

Then, the well-known algorithm for large symmetric complex matrices can be applied for solution of Eq. (56) with (58).

4.4 Modal Problems

We can find the resonance frequencies $f_k = \omega_k/(2\pi)$ for nanosized piezoelectric body using the finite element approaches from the solution of the generalized eigenvalue problem, obtained from (56) and (58) with $\mathbf{C}_{uu} = 0$, $\zeta_d = 0$, $\tilde{\mathbf{F}} = 0$, given by

$$\mathbf{K}_{uu} \cdot \tilde{\mathbf{U}} + \mathbf{K}_{u\varphi} \cdot \tilde{\boldsymbol{\Phi}} = \omega^2\mathbf{M}_{uu} \cdot \tilde{\mathbf{U}}, \tag{59}$$

$$-\mathbf{K}_{u\varphi}^T \cdot \tilde{\mathbf{U}} + \mathbf{K}_{\varphi\varphi} \cdot \tilde{\boldsymbol{\Phi}} = 0. \tag{60}$$

Eigenvalue problem (59) and (60) can be represented in the more compact form

$$\overline{\mathbf{K}}_{uu} \cdot \tilde{\mathbf{U}} = \omega^2 \mathbf{M}_{uu} \cdot \tilde{\mathbf{U}}, \tag{61}$$

where

$$\overline{\mathbf{K}}_{uu} = \mathbf{K}_{uu} + \mathbf{K}_{u\varphi} \cdot \mathbf{K}_{\varphi\varphi}^{-1} \cdot \mathbf{K}_{u\varphi}^{T}, \quad \tilde{\boldsymbol{\Phi}} = \mathbf{K}_{\varphi\varphi}^{-1} \cdot \mathbf{K}_{u\varphi}^{T} \cdot \tilde{\mathbf{U}}. \tag{62}$$

By virtue of positive definiteness of the intrinsic bulk and surface energies, the generalized stiffness matrix $\overline{\mathbf{K}}_{uu}$ is nonnegative definite ($\overline{\mathbf{K}}_{uu} \geq 0$), and mass matrix $\mathbf{M}_{uu}$ is positive definite ($\mathbf{M}_{uu} > 0$), because $\rho(\mathbf{x}) \geq \rho_0 > 0$. Then, by analogy with the classical eigenvalue problems for elastic body of usual size, the eigenvalues $\lambda_k = \omega_k^2$ ($k = 1, 2, \ldots, n$; n is the order of matrices $\overline{\mathbf{K}}_{uu}$ and $\mathbf{M}_{uu}$) are real and non-negative. The eigenvectors, corresponding to them, which we will denote by $\mathbf{W}_k = \tilde{\mathbf{U}}_k$, form basis in R^n. The system of these eigenvectors can be chosen orthonormal with respect to the mass matrix $\mathbf{M}_{uu}$ and orthogonal with respect to the generalized stiffness matrix $\overline{\mathbf{K}}_{uu}$

$$\langle \mathbf{W}_k, \mathbf{W}_m \rangle = \mathbf{W}_k^T \cdot \mathbf{M}_{uu} \cdot \mathbf{W}_m = \delta_{km}, \quad \mathbf{W}_k^T \cdot \overline{\mathbf{K}}_{uu} \cdot \mathbf{W}_m = \omega_m^2 \delta_{km}. \tag{63}$$

Thus, the coupled eigenvalue problems (59) and (60) with respect to the triple of unknowns $\{\omega, \tilde{\mathbf{U}}, \tilde{\boldsymbol{\Phi}}\}$ are the generalized eigenvalue problems (61) and (62) with respect to the pairs $\{\omega, \tilde{\mathbf{U}}\}$.

4.5 Mode Superposition Method for Steady-State Oscillation Problems

In the case of harmonic problem with $\beta_d = \zeta_d$ on solution of Eq. (56) with (58), we obtain

$$(-\omega^2 \mathbf{M}_{uu} + j\omega \overline{\mathbf{C}}_{uu} + \overline{\mathbf{K}}_{uu}) \cdot \tilde{\mathbf{U}} = \overline{\mathbf{F}}_u, \tag{64}$$

$$\overline{\mathbf{C}}_{uu} = \alpha_d \mathbf{M}_{uu} + \beta_d \overline{\mathbf{K}}_{uu}, \quad \overline{\mathbf{F}}_u = \tilde{\mathbf{F}}_u - \mathbf{K}_{u\varphi} \cdot \tilde{\boldsymbol{\Phi}}_{st}, \tag{65}$$

$$\tilde{\boldsymbol{\Phi}} = \tilde{\boldsymbol{\Phi}}_{st} + (1 + j\omega\beta_d) \mathbf{K}_{\varphi\varphi}^{-1} \cdot \mathbf{K}_{u\varphi}^{T} \cdot \tilde{\mathbf{U}}, \quad \tilde{\boldsymbol{\Phi}}_{st} = \mathbf{K}_{\varphi\varphi}^{-1} \cdot \tilde{\mathbf{F}}_{\varphi}. \tag{66}$$

If $\mathbf{u}_\Gamma = 0$ in (12), we will find the solution of problem (64) in the form of an expansion in eigenvectors (modes) $\mathbf{W}_k$ of eigenvalue problem (61) with the same homogeneous principal mechanical boundary conditions

$$\tilde{\mathbf{U}} = \sum_{k=1}^{n} z_k \mathbf{W}_k. \tag{67}$$

Substituting (67) into (64) and multiplying the obtained equation scalarly by $\mathbf{W}_m^*$ and taking into account the orthogonality relations (63) and (65), we obtain

$$z_k = \frac{1}{\omega_k^2 - \omega^2 + 2j\xi_k\omega_k\omega} P_k, \quad P_k = \mathbf{W}_k^T \cdot \overline{\mathbf{F}}_u, \quad \xi_k = \alpha_d \frac{1}{2\omega_k} + \beta_d \frac{\omega_k}{2}. \tag{68}$$

Thus, using the method of mode superposition, the solutions of the harmonic problems are determined by (66)–(68).

The advantages and disadvantages of the mode-expansion 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 (68). These factors can be specified from the experimentally measured value of the coupled mechanical and electric quality factor Q_k of the mode with number k: $\xi_k = 1/(2Q_k)$.

4.6 *Mode Superposition Method for Nonstationary Problems*

For transient problems with homogeneous principal boundary conditions and $\beta_d = \zeta_d$ we can also apply the method of mode superposition. Having solved Eq. (48) for $\boldsymbol{\Phi}$ and converted Eq. (47), we obtain

$$\mathbf{M}_{uu} \cdot \ddot{\mathbf{U}} + \overline{\mathbf{C}}_{uu} \cdot \dot{\mathbf{U}} + \overline{\mathbf{K}}_{uu} \cdot \mathbf{U} = \mathbf{F}_u - \mathbf{K}_{u\varphi} \cdot \boldsymbol{\Phi}_{qst}, \tag{69}$$

$$\boldsymbol{\Phi} = \boldsymbol{\Phi}_{qst} + \mathbf{K}_{\varphi\varphi}^{-1} \cdot \mathbf{K}_{u\varphi}^T \cdot (\mathbf{U} + \beta_d \dot{\mathbf{U}}), \tag{70}$$

where $\boldsymbol{\Phi}_{qst}$ is determined from the separate quasistatic problem

$$\boldsymbol{\Phi}_{qst} = \mathbf{K}_{\varphi\varphi}^{-1} \cdot \mathbf{F}_\varphi. \tag{71}$$

We will find the solution $\mathbf{U}$ of problem (69) in the form of an expansion in modes (67), where $z_k = z_k(t)$. Substituting this expansion into Eq. (69), multiplying the resulting equality scalarly by $\mathbf{W}_m^T$, and using the orthogonality relation (63), we derive scalar differential equations for the individual functions $z_k(t)$. Solving these equations with corresponding initial conditions, we obtain

$$z_k = \frac{1}{\overline{\omega}_k} \int_0^t P_k(\tau) e^{-\xi_k\omega_k(t-\tau)} \sin[\overline{\omega}_k(t-\tau)]\, d\tau + A_k(0) e^{-\xi_k\omega_k t} \sin(\overline{\omega}_k t + \delta_k), \tag{72}$$

$$P_k = \mathbf{W}_k^T \cdot (\mathbf{F}_u - \mathbf{K}_{u\varphi} \cdot \boldsymbol{\Phi}_{qst}), \quad \overline{\omega}_k = \omega_k \sqrt{1 - \xi_k^2}, \tag{73}$$

$$A_k(0) = \sqrt{z_k^2(0) + \frac{(\dot{z}_k(0) + \xi_k\omega_k z_k(0))^2}{\overline{\omega}_k^2}}, \quad \delta_k = \operatorname{arctg}\frac{z_k(0)\overline{\omega}_k}{\dot{z}_k(0) + \xi_k\omega_k z_k(0)}, \tag{74}$$

$$z_k(0) = \mathbf{W}_k^T \cdot \mathbf{M}_{uu} \cdot \mathbf{U}_*, \quad \dot{z}_k(0) = \mathbf{W}_k^T \cdot \mathbf{M}_{uu} \cdot \mathbf{R}_*. \tag{75}$$

Hence, using mode superposition method, the solution of problem (47) and (48) with homogeneous principal mechanical boundary conditions and $\beta_d = \zeta_d$ is given by (67) and (72)–(75) for $\mathbf{U}$ and by (70) and (71) for $\boldsymbol{\Phi}$.

4.7 The Newmark Scheme for Solving Non-stationary Problems

The mode superposition method requires the equality of the damping parameters for different media and the homogeneity of the principal boundary conditions. Methods of direct integration with respect to time are more general. We will use the Newmark method for integrating Cauchy problem (47)–(49) in a formulation in which the velocities and accelerations in the time layers are not explicitly given [50].

This variant of the Newmark scheme base on the average expressions on time layer t_i for the vector functions $\mathbf{a}_i = \mathbf{a}(t_i)$, $\mathbf{a} = \{\mathbf{U}, \boldsymbol{\Phi}\}$ and its derivatives ($t_i = i\tau$, $\tau = \Delta t$ is the constant time step size)

$$\mathbf{a}_i \approx \beta\mathbf{a}_{j+1} + \beta_1\mathbf{a}_j + \beta_2\mathbf{a}_{j-1}, \tag{76}$$

$$\dot{\mathbf{a}}_i \approx (\gamma\mathbf{a}_{i+1} + \gamma_1\mathbf{a}_i + \gamma_2\mathbf{a}_{i-1})/\tau, \tag{77}$$

$$\ddot{\mathbf{a}}_i \approx (\mathbf{a}_{i+1} - 2\mathbf{a}_i + \mathbf{a}_{i-1})/\tau^2, \tag{78}$$

where $\beta_1 = 1/2 + \gamma - 2\beta$, $\beta_2 = 1/2 - \gamma + \beta$, $\gamma_1 = 1 - 2\gamma$, $\gamma_2 = \gamma - 1$, β and γ are the parameters of the Newmark method.

Writing Eqs. (47) and (48) for the time layer t_i, and using representations (76)–(78), we obtain the system of linear equations for $\mathbf{a}_{i+1}$, if we count the known values at the previous time layers t_i and t_{i-1}

$$\mathbf{K}^{\text{eff}} \cdot \mathbf{a}_{i+1} = \mathbf{F}_{i+1}^{\text{eff}}(\mathbf{a}_i, \mathbf{a}_{i-1}), \tag{79}$$

where

$$\mathbf{K}^{\text{eff}} = \begin{bmatrix} \mathbf{K}_{uu}^{\text{eff}} & \mathbf{K}_{u\varphi} \\ \mathbf{K}_{u\varphi}^T & -\lambda\mathbf{K}_{\varphi\varphi} \end{bmatrix}, \quad \mathbf{a}_{i+1} = \begin{bmatrix} \mathbf{U}_{i+1} \\ \boldsymbol{\Phi}_{i+1} \end{bmatrix}, \quad \mathbf{F}^{\text{eff}} = \begin{bmatrix} \mathbf{F}_{u,i+1}^{\text{eff}} \\ -\mathbf{F}_{\varphi,i+1}^{\text{eff}} \end{bmatrix}, \tag{80}$$

$$\mathbf{K}_{uu}^{\text{eff}} = \mathbf{K}_{uu} + \frac{\gamma}{\beta\tau}\mathbf{C}_{uu} + \frac{1}{\beta\tau^2}\mathbf{M}_{uu}, \quad \lambda = (1 + \frac{\zeta_d\gamma}{\beta\tau})^{-1}, \tag{81}$$

$$\mathbf{F}_{u,i+1}^{\text{eff}} = \mathbf{F}_{u,i+1} + \frac{\beta_1}{\beta}\mathbf{F}_{u,i} + \frac{\beta_2}{\beta}\mathbf{F}_{u,i-1} - (\frac{\beta_1}{\beta}\mathbf{K}_{uu} + \frac{\gamma_1}{\beta\tau}\mathbf{C}_{uu} - \frac{2}{\beta\tau^2}\mathbf{M}_{uu}) \cdot \mathbf{U}_i - \tag{82}$$

$$-(\frac{\beta_2}{\beta}\mathbf{K}_{uu} + \frac{\gamma_2}{\beta\tau}\mathbf{C}_{uu} + \frac{1}{\beta\tau^2}\mathbf{M}_{uu}) \cdot \mathbf{U}_{i-1} - \frac{\beta_1}{\beta}\mathbf{K}_{uu} \cdot \boldsymbol{\Phi}_i - \frac{\beta_2}{\beta}\mathbf{K}_{uu} \cdot \boldsymbol{\Phi}_{i-1},$$

$$\mathbf{F}_{\varphi,i+1}^{\text{eff}} = \lambda\mathbf{F}_{\varphi,i+1} + \frac{\lambda\beta_1}{\beta}\mathbf{F}_{\varphi,i} + \frac{\lambda\beta_2}{\beta}\mathbf{F}_{\varphi,i-1} + \frac{\lambda(\beta_1 + \zeta_d\gamma_1)}{\beta\tau}\mathbf{K}_{u\varphi}^T \cdot \mathbf{U}_i + \tag{83}$$

$$+\frac{\lambda(\beta_2 + \zeta_d\gamma_2)}{\beta\tau}\mathbf{K}_{u\varphi}^T \cdot \mathbf{U}_{i-1} - \frac{\lambda\beta_1}{\beta}\mathbf{K}_{\varphi\varphi}^T \cdot \boldsymbol{\Phi}_i - \frac{\lambda\beta_2}{\beta}\mathbf{K}_{\varphi\varphi}^T \cdot \boldsymbol{\Phi}_{i-1}.$$

The matrix $\mathbf{K}^{\text{eff}}$ can be factorized using the LDL^T–factorization method, and only the systems of linear algebraic equations with lower and upper triangular matrices can be solved in each time layer.

Note that the Newmark scheme is absolutely stable when $\beta \geq (1/2 + \gamma)^2/4$; $\gamma \geq 1/2$, and, when $\beta \geq 1/4$; $\gamma = 1/2$, it does not have an approximation viscosity [50]. The Newmark scheme in form (79)–(83) does not explicitly use velocities and accelerations, and this makes it preferable in the case of the transient problems for piezoelectric nanosized solids with account for coupled damping and surface effects.

5 Concluding Remarks

Thus, we have proposed a new model that describes the behavior of the piezoelectric materials, taking into account the damping properties and surface effects at the nanoscale.

The novelty of the model consists in taking into account the volumetric and surface damping properties, as well as coupled surface material phenomena which are important at the nanoscale. To describe the size effects, we use recently popular theory of surface stresses and its generalization to piezoelectric media. Under this generalization, we also consider the coupled surface mechanical and electric fields. Other new feature is the account for the damping properties in the sense of a generalization of the conventional for the structural analysis Rayleigh damping method for the coupled mechanical and electric fields. We also added the terms, describing the attenuation, in the constitutive equations for the surface mechanic and electric fields. When taking the coupled damping into account, the basic idea was that the method of mode superposition can be applied for transient and harmonic problems for piezoelectric bodies at the nanoscale.

After the initial-boundary value problem setting for the piezoelectric nanosized bodies, we have obtained a weak or generalized formulation of this problem in terms