

CONTINUAL AND FINITE ELEMENT MODELLING OF ELECTRICALLY ACTIVE MATERIALS WITH MICROSTRUCTURE AND SURFACE EFFECTS

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Abstract: *The paper considers the dynamic problems for magnetolectric (piezomagnetolectric) nanodimensional bodies with account for surface mechanical, electric and magnetic effects. For transient problem the new mathematical model is suggested, which generalize the model of the elastic medium with damping properties and surface effects for the cases of piezoelectric and magnetolectric materials. For solving these problems the finite element approximations are proposed. The paper also deals with computer design of multiscale two-phase magnetolectric bulk composites that consist of piezomagnetic and piezoelectric fractions of regular and irregular structures, modeling of the representative volumes, taking into account for microstructure features, using the finite element technologies for solving the problems for the representative volumes.*

1 INTRODUCTION

Electrically active materials (piezoelectric and magnetolectric materials) are widely used for the manufacture of high-tech devices for medical diagnostics and therapy, hydroacoustics, nondestructive testing and diagnostics, level and flow metering, consumer, automotive, biomedical and aerospace industries. Rapidly growing demand for efficiency, reliability and cost constantly stimulates the development of new and improved materials, devices and systems. The analysis shows that the properties of the electrically active material remain the limiting factor in the development of more effective piezoelectric transducers and devices. The simulation and experimental studies of electrically active materials at various scale levels help to enhance the technologies of directed changing of the properties of these materials and provide a qualitative improvement of their characteristics. The developed in the recent years new nanostructured electrically active materials and composites have a range of important advantages, such as the possibilities of controllable variation of the functional characteristics within a wide range, the ultra-low mechanical quality factor, the large electromechanical anisotropy, the giant dielectric relaxation, and the electrocaloric and piezoelectric effects.

Furthermore, it should be noted that the modeling of micro- and nanomaterials and devices has some specific features. It is known that a range of nanomaterials have abnormal mechanical properties that considerably differ from the properties of ordinary macrosized bodies. Thus, the experimentally observed fact is the increasing of the stiffness with reducing the sizes of nanoobjects. One of the factors that are responsible for this behavior of nanomaterials can be surface effects. As research of the recent years shows, for the bodies of submicro- and nanosizes the surface stresses play an important role and influence the deformation of the bodies in general [6, 7, 8, 25]. In connection to this, the actual problem can be an extension of this approach to the nanoscale elements of electrically active composites and materials [10, 23, 26, 27]. Therefore, here it is logical to consider not only the mechanical surface effects, but also for the surface effects of electric and magnetic fields.

In present investigation in Sect. 2 we develop the models of electrically active materials account for their internal microstructure in the framework of classic continuum approaches of solid mechanics and methods of composite mechanics. We use these models to construct new models of the micro- and nanosize bodies made of electrically active materials that were additionally take into account the surface and micro local effects [18, 19, 22].

In Sect. 3 we propose the finite element approximations for numerical solution of the formulated transient problems [?, 22]. We note that for solving the received finite element systems we can use the algorithms with symmetric quasidefinite matrices (matrices of saddle structure) [4]. This allows us to use corresponding effective direct and iterative solvers for systems with symmetric quasidefinite matrices for both static and transient problems [4, 9, 12, 29].

In Sect. 4, 5 we develop the effective moduli method and the finite element technique for magnetoelectric and piezoelectric composites [15, 16, 17].

2 DYNAMIC PROBLEM FOR MAGNETOELECTRIC BODY WITH SURFACE EFFECTS

Here we consider the bulk magnetostrictive – piezoelectric composites as the continuous magnetoelectric (piezo-magnetoelectric) material with effective properties defined by some homogeneous procedure, as for example described in [5, 11, 13, 28] and in Sect. 4.

Let $\Omega \in \mathbb{R}^3$ be a region occupied by a magnetoelectric material; $\Gamma = \partial\Omega$ is the boundary of Ω ; \mathbf{n} is the external unit normal to Γ ; $\mathbf{x} = \{x_1, x_2, x_3\}$; t is time; $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ is the vector of mechanical displacements; $\varphi = \varphi(\mathbf{x}, t)$ is the function of electric potential; $\phi = \phi(\mathbf{x}, t)$ is the function of magnetic potential. The system of differential equations for magnetoelectric body with damping effects in the volume Ω can be written in the following vector-matrix form:

$$\mathbf{L}^*(\nabla) \cdot \mathbf{T} + \rho \mathbf{f} = \rho (\ddot{\mathbf{u}} + \alpha_d \dot{\mathbf{u}}), \quad \nabla \cdot \mathbf{D} = \sigma_\Omega, \quad \nabla \cdot \mathbf{B} = 0, \quad (1)$$

$$\mathbf{T} = \mathbf{c} \cdot (\mathbf{S} + \beta_d \dot{\mathbf{S}}) - \mathbf{e}^* \cdot \mathbf{E} - \mathbf{h}^* \cdot \mathbf{H}, \quad (2)$$

$$\mathbf{D} + \zeta_d \dot{\mathbf{D}} = \mathbf{e} \cdot (\mathbf{S} + \zeta_d \dot{\mathbf{S}}) + \boldsymbol{\kappa} \cdot \mathbf{E} + \boldsymbol{\alpha} \cdot \mathbf{H}, \quad (3)$$

$$\mathbf{B} + \gamma_d \dot{\mathbf{B}} = \mathbf{h} \cdot (\mathbf{S} + \gamma_d \dot{\mathbf{S}}) + \boldsymbol{\alpha}^* \cdot \mathbf{E} + \boldsymbol{\mu} \cdot \mathbf{H}, \quad (4)$$

$$\mathbf{S} = \mathbf{L}(\nabla) \cdot \mathbf{u}, \quad \mathbf{E} = -\nabla\varphi, \quad \mathbf{H} = -\nabla\phi, \quad (5)$$

$$\mathbf{L}^*(\nabla) = \begin{bmatrix} \partial_1 & 0 & 0 & 0 & \partial_3 & \partial_2 \\ 0 & \partial_2 & 0 & \partial_3 & 0 & \partial_1 \\ 0 & 0 & \partial_3 & \partial_2 & \partial_1 & 0 \end{bmatrix}. \quad (6)$$

Here $\mathbf{T} = \{\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{23}, \sigma_{13}, \sigma_{12}\}$; $\mathbf{S} = \{\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, 2\varepsilon_{23}, 2\varepsilon_{13}, 2\varepsilon_{12}\}$; σ_{ij} and ε_{ij} are the components of the second-order stress and strain tensors, respectively; \mathbf{D} is the electric flux density vector called also the electric displacement vector; \mathbf{E} is the electric field vector; \mathbf{B} is the magnetic field vector; \mathbf{H} is the magnetic flux density vector; $\mathbf{c} = \mathbf{c}^{E,H}$ is the 6×6 matrix of elastic stiffness moduli; $\mathbf{e} = \mathbf{e}^H$ is the 3×6 matrix of piezoelectric moduli; $\mathbf{h} = \mathbf{h}^E$ is the 3×6 matrix of magnetostriction moduli (piezomagnetic moduli); $\boldsymbol{\kappa} = \boldsymbol{\kappa}^{S,H} = \boldsymbol{\epsilon}^{S,H}$ is the 3×3 matrix of dielectric permittivity moduli; $\boldsymbol{\alpha} = \boldsymbol{\alpha}^S$ is the 3×3 matrix of magnetoelectric coupling coefficients; $\boldsymbol{\mu} = \boldsymbol{\mu}^{S,E}$ is the 3×3 matrix of magnetic permeability moduli. The upper indexes indicate the constant fields under which these moduli are calculated. So S denotes the strains, E denotes the electric field, H denotes the magnetic field. $\alpha_d, \beta_d, \zeta_d, \gamma_d$ are the damping coefficients; \mathbf{f} is the vector of mass forces; σ_Ω is the density of free electric charges (usually, $\sigma_\Omega = 0$); $(\dots)^*$ is the transpose operation, and $(\dots) \cdot (\dots)$ is the scalar product operation.

We suppose that the material moduli have the usual symmetry properties: $c_{\alpha\beta} = c_{\beta\alpha}$, $\kappa_{kl} = \kappa_{lk}$, $\mu_{kl} = \mu_{lk}$. In addition to the latter the requirement of positive definiteness of the intrinsic energy of the magnetoelectric medium leads to the following inequalities valid for all \mathbf{S} , $\varepsilon_{ij} = \varepsilon_{ji}$, \mathbf{E} and \mathbf{H} :

$$\mathbf{S}^* \cdot \mathbf{c} \cdot \mathbf{S} + \mathbf{E}^* \cdot \boldsymbol{\kappa} \cdot \mathbf{E} + 2\mathbf{E}^* \cdot \boldsymbol{\alpha} \cdot \mathbf{H} + \mathbf{H}^* \cdot \boldsymbol{\mu} \cdot \mathbf{H} \geq c_{vU} (\mathbf{S}^* \cdot \mathbf{S} + \mathbf{E}^* \cdot \mathbf{E} + \mathbf{H}^* \cdot \mathbf{H}),$$

where $c_{vU} > 0$ is a positive constant.

In models (1)–(6) for the magnetoelectric material, we use a generalized Rayleigh method of damping evaluation, see [3, 14] for the case of piezoelectric material, which is admissible for many practical applications. When $\zeta_d = \gamma_d = 0$ in Eqs. (3) and (4), we have the model for taking into account of mechanical damping in magnetoelectric media which is adopted in the case of elastic and piezoelectric materials in several well-known finite element packages. More complicated model (3) and (4) extends Kelvin's model to the case of magnetoelectric media. It has been shown that the model (1)–(6) with $\beta_d = \zeta_d = \gamma_d$ 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 piezomagnetoelectric media.

For completeness the boundary and the initial conditions should be added to the system of differential equations (1)–(6). The boundary conditions are of three types: mechanical, electric and magnetic.

To formulate the mechanical boundary conditions we assume that the boundary $\Gamma \equiv \partial\Omega$ is divided in two subsets Γ_σ and Γ_u ($\Gamma = \Gamma_\sigma \cup \Gamma_u$) for dynamic and kinematic boundary conditions, respectively. The dynamic boundary conditions given at Γ_σ take the form

$$\mathbf{L}^*(\mathbf{n}) \cdot \mathbf{T} = \mathbf{L}^*(\nabla^s) \cdot \boldsymbol{\tau}^s + \mathbf{p}_\Gamma, \quad \mathbf{x} \in \Gamma_\sigma, \quad (7)$$

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 along the direction of normal \mathbf{n} to Γ_σ ; $\boldsymbol{\tau}^s = \{\sigma_{11}^s, \sigma_{22}^s, \sigma_{33}^s, \sigma_{23}^s, \sigma_{13}^s, \sigma_{12}^s\}$; σ_{ij}^s are the components of the second-order tensor of surface stresses, and \mathbf{p}_Γ is the external surface loads.

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 $\boldsymbol{\varepsilon}^s = \{\varepsilon_{11}^s, \varepsilon_{22}^s, \varepsilon_{33}^s, 2\varepsilon_{23}^s, 2\varepsilon_{13}^s, 2\varepsilon_{12}^s\}$ by the formula $\boldsymbol{\tau}^s = \mathbf{c}^s \cdot (\boldsymbol{\varepsilon}^s + \beta_d \dot{\boldsymbol{\varepsilon}}^s)$, where $\boldsymbol{\varepsilon}^s = \mathbf{L}(\nabla^s) \cdot (\mathbf{u} \cdot \mathbf{A})$; \mathbf{c}^s is the 6×6 matrix of surface elastic moduli; $\mathbf{A} = \mathbf{I} - \mathbf{n} \otimes \mathbf{n}$; \mathbf{I} is the unit tensor (3×3 matrix) in \mathbb{R}^3 .

Here the properties of the matrix of surface elastic modules \mathbf{c}^s are analogous to the corresponding properties of the matrix \mathbf{c} , i.e. $c_{\alpha\beta}^s = c_{\beta\alpha}^s$,

$$\exists c_s U > 0, \quad \forall \boldsymbol{\varepsilon}^s, \varepsilon_{ij}^s = \varepsilon_{ji}^s : \quad U(\boldsymbol{\varepsilon}^s) = \frac{1}{2} \boldsymbol{\varepsilon}^{s*} \cdot \mathbf{c}^s \cdot \boldsymbol{\varepsilon}^s \geq c_s U \boldsymbol{\varepsilon}^{s*} \cdot \boldsymbol{\varepsilon}^s,$$

that follow from the condition of the positive definiteness of the surface energy density $U(\boldsymbol{\varepsilon}^s)$ which is required for well-posedness of the problem [1].

On the remaining part Γ_u of boundary Γ we pose known the mechanical displacements vector \mathbf{u}_Γ

$$\mathbf{u} = \mathbf{u}_\Gamma, \quad \mathbf{x} \in \Gamma_u. \quad (8)$$

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, so the following conditions hold

$$\mathbf{n} \cdot \mathbf{D} = \nabla^s \cdot \mathbf{d}^s - \sigma_\Gamma, \quad \mathbf{x} \in \Gamma_D, \quad (9)$$

where the surface electric flux density vector \mathbf{d}^s joins with the surface electric field vector $\mathbf{E}^s = -\nabla^s \varphi$ by the constitutive equation $\mathbf{d}^s + \zeta_d \dot{\mathbf{d}}^s = \mathbf{A} \cdot \boldsymbol{\kappa}^s \cdot \mathbf{A} \cdot \mathbf{E}^s$; $\boldsymbol{\kappa}^s$ is the dielectric surface permittivity 3×3 matrix that is symmetric positive definite relatively to the vectors \mathbf{E}^s ; σ_Γ is the given surface density of electric charge, and usually, $\sigma_\Gamma = 0$.

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

$$\varphi = \Phi_j, \quad \mathbf{x} \in \Gamma_{\varphi j}, \quad j \in J_Q, \quad (10)$$

$$\int_{\Gamma_{\varphi j}} \mathbf{n} \cdot \mathbf{D} d\Gamma = -Q_j, \quad I_j = \pm \dot{Q}_j, \quad \mathbf{x} \in \Gamma_{\varphi j}, \quad j \in J_Q, \quad (11)$$

$$\varphi = V_j, \quad \mathbf{x} \in \Gamma_{\varphi j}, \quad j \in J_V, \quad \Gamma_{j0} \neq \emptyset, \quad (12)$$

where the variables Φ_j, V_j do not depend on \mathbf{x} ; Q_j is the overall electric charge on $\Gamma_{\varphi j}$, and the sign “ \pm ” in (11) is chosen in accordance with the accepted direction of the current I_j in the electric circuit.

For magnetic boundary condition we suppose that the following condition hold on boundary Γ

$$\mathbf{n} \cdot \mathbf{B} = \nabla^s \cdot \mathbf{b}^s, \quad \mathbf{x} \in \Gamma, \quad (13)$$

where the surface magnetic flux density vector \mathbf{b}^s depends from the surface magnetic field vector $\mathbf{H}^s = -\nabla^s \phi$ by the constitutive equation $\mathbf{b}^s + \gamma_d \dot{\mathbf{b}}^s = \mathbf{A} \cdot \boldsymbol{\mu}^s \cdot \mathbf{A} \cdot \mathbf{H}^s$; $\boldsymbol{\mu}^s$ is the magnetic surface permittivity 3×3 matrix that is symmetric positive definite relatively to the vectors \mathbf{H}^s .

For transient problems it is also necessary to pose initial conditions which are given by

$$\mathbf{u} = \mathbf{u}_*(\mathbf{x}), \quad \dot{\mathbf{u}} = \mathbf{v}_*(\mathbf{x}), \quad t = 0, \quad \mathbf{x} \in \Omega, \quad (14)$$

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

Formulas (1)–(14) represent the statement of the transient problem for magnetoelectric body with the generalized Rayleigh damping and with account for surface effects for mechanical, electric and magnetic fields. From (1)–(14) we can also obtain the formulations of static, modal and harmonic problems for magnetoelectric media with surface effects by standard methods.

We can also consider the particular cases of this model without tacking into account the connectivity between some physical fields, and without the surface mechanical stresses ($\boldsymbol{\tau}^s = 0$), surface electric fields ($\mathbf{d}^s = 0$), or surface magnetic fields ($\mathbf{b}^s = 0$).

For example, we can obtain the model of piezoelectric material with damping properties and with surface effects, if we assume $\mathbf{h} = 0$ in (2), $\boldsymbol{\alpha} = 0$ in (3) and if we ignore the equations for magnetic fields.

3 FINITE ELEMENT APPROXIMATIONS

For solving the problems (1)–(14) we shall use the classical finite element approximation techniques [2, 30]. Let Ω_h be the region of the corresponding finite element mesh: $\Omega_h \subseteq \Omega$, $\Omega_h = \cup_m \Omega^{em}$. On this mesh we shall find the approximation to the weak solution $\{\mathbf{u}_h \approx \mathbf{u}, \varphi_h \approx \varphi, \phi_h\} \approx \phi$ in the form

$$\mathbf{u}_h(\mathbf{x}, t) = \mathbf{N}_u^*(\mathbf{x}) \cdot \mathbf{U}(t), \quad \varphi_h(\mathbf{x}, t) = \mathbf{N}_\varphi^*(\mathbf{x}) \cdot \Phi(t), \quad \phi_h(\mathbf{x}, t) = \mathbf{N}_\phi^*(\mathbf{x}) \cdot \Psi(t), \quad (15)$$

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

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

$$\mathbf{v}(\mathbf{x}) = \mathbf{N}_u^*(\mathbf{x}) \cdot \delta \mathbf{U}, \quad \chi(\mathbf{x}) = \mathbf{N}_\varphi^*(\mathbf{x}) \cdot \delta \Phi, \quad \eta(\mathbf{x}) = \mathbf{N}_\phi^*(\mathbf{x}) \cdot \delta \Psi. \quad (16)$$

In accordance with standard finite element technique we approximate the weak formulation of the problems (1)–(14) in finite-dimensional spaces. Substituting (15) and (16) into the weak formulation of the problems (1)–(14) for Ω_h , $\Gamma_h = \partial\Omega_h$, $\Gamma_{\sigma h}$, Γ_{Dh} , without taking into account the principal boundary conditions we obtain

$$\mathbf{M}_{uu} \cdot \ddot{\mathbf{U}} + \mathbf{C}_{uu} \cdot \dot{\mathbf{U}} + \mathbf{K}_{uu} \cdot \mathbf{U} + \mathbf{K}_{u\varphi} \cdot \Phi + \mathbf{K}_{u\phi} \cdot \Psi = \mathbf{F}_u, \quad (17)$$

$$-\mathbf{K}_{u\varphi}^* \cdot (\mathbf{U} + \zeta_d \dot{\mathbf{U}}) + \mathbf{K}_{\varphi\varphi} \cdot \Phi + \mathbf{K}_{\varphi\phi} \cdot \Psi = \mathbf{F}_\varphi, \quad (18)$$

$$-\mathbf{K}_{u\phi}^* \cdot (\mathbf{U} + \gamma_d \dot{\mathbf{U}}) + \mathbf{K}_{\varphi\phi}^* \cdot \Phi + \mathbf{K}_{\phi\phi} \cdot \Psi = 0, \quad (19)$$

with the initial conditions

$$\mathbf{U}(0) = \mathbf{U}_*, \quad \dot{\mathbf{U}}(0) = \mathbf{V}_*, \quad (20)$$

which are derived from the corresponding conditions (14).

Here, $\mathbf{M}_{uu} = \sum^a \mathbf{M}_{uu}^{ek}$, $\mathbf{C}_{uu} = \sum^a \mathbf{C}_{uu}^{ek}$, $\mathbf{K}_{uu} = \sum^a \mathbf{K}_{uu}^{ek}$, $\mathbf{K}_{u\varphi} = \sum^a \mathbf{K}_{u\varphi}^{ek}$, etc., are the global matrices, obtained from the corresponding element matrices ensemble (\sum^a).

The element matrices are given by the formulas

$$\mathbf{M}_{uu}^{ek} = \int_{\Omega^{ek}} \rho \mathbf{N}_u^e \cdot \mathbf{N}_u^{e*} d\Omega, \quad \mathbf{C}_{uu}^{ek} = \alpha_d \mathbf{M}_{uu}^{ek} + \beta_d \mathbf{K}_{uu}^{ek}, \quad (21)$$

$$\mathbf{K}_{uu}^{ek} = \mathbf{K}_{\Omega uu}^{ek} + \mathbf{K}_{\Gamma uu}^{ek}, \quad \mathbf{K}_{\varphi\varphi}^{ek} = \mathbf{K}_{\Omega\varphi\varphi}^{ek} + \mathbf{K}_{\Gamma\varphi\varphi}^{ek}, \quad \mathbf{K}_{\phi\phi}^{ek} = \mathbf{K}_{\Omega\phi\phi}^{ek} + \mathbf{K}_{\Gamma\phi\phi}^{ek}, \quad (22)$$

$$\mathbf{K}_{\Omega uu}^{ek} = \int_{\Omega^{ek}} \mathbf{B}_u^{e*} \cdot \mathbf{c} \cdot \mathbf{B}_u^e d\Omega, \quad \mathbf{K}_{\Gamma uu}^{ek} = \int_{\Gamma_{\sigma^{ek}}} \mathbf{B}_{su}^{e*} \cdot \mathbf{c}^s \cdot \mathbf{B}_{su}^e d\Gamma, \quad (23)$$

$$\mathbf{K}_{\Omega\varphi\varphi}^{ek} = \int_{\Omega^{ek}} \mathbf{B}_{\varphi}^{e*} \cdot \boldsymbol{\kappa} \cdot \mathbf{B}_{\varphi}^e d\Omega, \quad \mathbf{K}_{\Gamma\varphi\varphi}^{ek} = \int_{\Gamma_D^{ek}} \mathbf{B}_{s\varphi}^{e*} \cdot \boldsymbol{\kappa}^s \cdot \mathbf{B}_{s\varphi}^e d\Gamma, \quad (24)$$

$$\mathbf{K}_{\Omega\phi\phi}^{ek} = \int_{\Omega^{ek}} \mathbf{B}_{\phi}^{e*} \cdot \boldsymbol{\mu} \cdot \mathbf{B}_{\phi}^e d\Omega, \quad \mathbf{K}_{\Gamma\phi\phi}^{ek} = \int_{\Gamma^{ek}} \mathbf{B}_{s\phi}^{e*} \cdot \boldsymbol{\mu}^s \cdot \mathbf{B}_{s\phi}^e d\Gamma, \quad (25)$$

$$\mathbf{K}_{u\varphi}^{ek} = \int_{\Omega^{ek}} \mathbf{B}_u^{e*} \cdot \mathbf{e}^* \cdot \mathbf{B}_{\varphi}^e d\Omega, \quad \mathbf{K}_{u\phi}^{ek} = \int_{\Omega^{ek}} \mathbf{B}_u^{e*} \cdot \mathbf{h}^* \cdot \mathbf{B}_{\phi}^e d\Omega, \quad (26)$$

$$\mathbf{K}_{\varphi\phi}^{ek} = \int_{\Omega^{ek}} \mathbf{B}_{\varphi}^{e*} \cdot \boldsymbol{\alpha} \cdot \mathbf{B}_{\phi}^e d\Omega, \quad (27)$$

$$\mathbf{B}_{(s)u}^e = \mathbf{L}(\nabla^{(s)}) \cdot \mathbf{N}_u^{e*}, \quad \mathbf{B}_{(s)\varphi}^e = \nabla^{(s)} \mathbf{N}_{\varphi}^{e*}, \quad \mathbf{B}_{(s)\phi}^e = \nabla^{(s)} \mathbf{N}_{\phi}^{e*}, \quad (28)$$

where Γ^{ek} , Γ_{σ}^{ek} , Γ_D^{ek} , are the edges of finite elements facing the regions Γ_h , $\Gamma_{h\sigma}$, Γ_{hD} , that approximate the corresponding boundaries Γ , Γ_{σ} , Γ_{hD} ; \mathbf{N}_u^{e*} , $\mathbf{N}_{\varphi}^{e*}$, \mathbf{N}_{ϕ}^{e*} are the matrices and the row vectors of approximate shape functions, respectively, defined on separate finite elements.

We note that in (17)–(28) 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 mechanical force vector \mathbf{F}_u are formed in the same way as for purely elastic body, the matrices $\mathbf{K}_{u\varphi}$, $\mathbf{K}_{u\varphi}^{ek}$, $\mathbf{K}_{\Omega\varphi\varphi}$, $\mathbf{K}_{\Omega\varphi\varphi}^{ek}$ and nodal electric force vector \mathbf{F}_{φ} are identical to the corresponding matrices and vector for piezoelectric bodies, and $\mathbf{K}_{u\phi}$, $\mathbf{K}_{u\phi}^{ek}$, $\mathbf{K}_{\Omega\phi\phi}$, $\mathbf{K}_{\Omega\phi\phi}^{ek}$ are identical to the corresponding matrices for piezomagnetic bodies. The vectors \mathbf{F}_u and \mathbf{F}_{φ} in (17), (18) are obtained from the boundary conditions, the corresponding right parts of the weak statements, and the finite element approximations. The matrices $\mathbf{K}_{\Gamma uu}$, $\mathbf{K}_{\Gamma uu}^{ek}$, $\mathbf{K}_{\Gamma\varphi\varphi}$, $\mathbf{K}_{\Gamma\varphi\varphi}^{ek}$ and $\mathbf{K}_{\Gamma\phi\phi}$, $\mathbf{K}_{\Gamma\phi\phi}^{ek}$ are defined by the surface stresses and surface electric and magnetic films, respectively. These matrices are analogous to the stiffness matrices for surface elastic membranes and the matrices of dielectric and magnetic permittivities for surface dielectric and magnetic films. Hence, for implementing the finite element magnetoelectric analysis for the bodies with surface effects it is necessary to have surface structural membrane elements and surface finite elements of dielectric and magnetic films along with ordinary solid magnetoelectric finite elements.

For the case of the homogeneous principal boundary conditions with $\beta_d = \zeta_d = \gamma_d$, we can apply the mode superposition method for solving harmonic and transient problems. The given fact is one of the primary preference for the selected method for damping account and the supplement of the terms with β_d , ζ_d and γ_d in constitutive equations for volumetric and surface fields.

Note that similarly to [3, 14] we can use an effective algorithm with symmetric quasidefinite matrices for solving finite element Eqs. (17)–(19). For example we can use Newmark method for integrating Cauchy problem (17)–(20) with symmetric quasidefinite effective stiffness matrices in a formulation where the velocities and the accelerations at the time layers are not given explicitly [3, 14]. All the procedures that we need in finite element manipulations (the degree of freedom rotations, mechanical and electric boundary condition settings, etc.) we can also provide in a symmetric form.

4 MODELS OF MAGNETOELECTRIC COMPOSITE MATERIALS

Now, let Ω be a volume of two-phase composite heterogeneous body composed of two materials Ω_e and Ω_m ($\Omega = \Omega_e \cup \Omega_m$), where the phase Ω_e has the piezoelectric properties and the phase Ω_m has the piezomagnetic properties. Both phases Ω_e and Ω_m can consist of separate, generally speaking, disjointed subregions $\Omega_e = \cup_k \Omega_{ek}$, $\Omega_m = \cup_l \Omega_{ml}$, that in the aggregate have common boundaries and do not overlap each other. Thus, here we consider a two-phase mixture composite with piezoelectric and piezomagnetic fractions.

As usual, we will denote the volume-averaged quantities in the broken brackets as:

$$\langle\langle(\dots)\rangle\rangle = \frac{1}{|\Omega|} \int_{\Omega} (\dots) d\Omega. \quad (29)$$

We will formulate the auxiliary statements for electromagnetoelastic body [15, 16, 17] following the proof of the effective moduli method for elastic medium. These statements are substantiated under similar techniques, that are used for elastic and piezoelectric bodies [20, 24].

Lemma 1. These representations take place for the field characteristics (5) averaged in the volume Ω by means of the appropriate values on the boundary Γ :

$$(a) \quad \forall \mathbf{S}, \quad \langle S_j \rangle = \frac{1}{|\Omega|} \int_{\Gamma} u_j n_j d\Gamma, \quad j = 1, 2, 3, \quad \langle S_4 \rangle = \frac{1}{|\Omega|} \int_{\Gamma} (u_2 n_3 + u_3 n_2) d\Gamma,$$

$$\langle S_5 \rangle = \frac{1}{|\Omega|} \int_{\Gamma} (u_1 n_3 + u_3 n_1) d\Gamma, \quad \langle S_6 \rangle = \frac{1}{|\Omega|} \int_{\Gamma} (u_1 n_2 + u_2 n_1) d\Gamma,$$

$$(b) \quad \forall \mathbf{E}, \mathbf{H}, \quad \langle \mathbf{E} \rangle = -\frac{1}{|\Omega|} \int_{\Gamma} \mathbf{n} \varphi d\Gamma, \quad \langle \mathbf{H} \rangle = -\frac{1}{|\Omega|} \int_{\Gamma} \mathbf{n} \phi d\Gamma.$$

Lemma 2. For $\mathbf{x} \in \Gamma$ we have the following relations:

(a) if $\mathbf{u} = \mathbf{L}^*(\mathbf{x}) \cdot \mathbf{S}_0$, where $\mathbf{S}_0 = \text{const}$, i.e. \mathbf{S}_0 consists of the components of arbitrary symmetric independent on \mathbf{x} second rank strain tensor, then $\langle \mathbf{S} \rangle = \mathbf{S}_0$;

(b) if $\varphi = -\mathbf{x} \cdot \mathbf{E}_0$, where $\mathbf{E}_0 = \text{const}$, i.e. \mathbf{E}_0 is the arbitrary independent on \mathbf{x} vector, then $\langle \mathbf{E} \rangle = \mathbf{E}_0$;

(c) if $\phi = -\mathbf{x} \cdot \mathbf{H}_0$, where $\mathbf{H}_0 = \text{const}$, i.e. \mathbf{H}_0 is the arbitrary independent on \mathbf{x} vector, then $\langle \mathbf{H} \rangle = \mathbf{H}_0$.

Lemma 3. If for $\mathbf{x} \in \Gamma$:

(a) $\mathbf{u} = \mathbf{L}^*(\mathbf{x}) \cdot \mathbf{S}_0$, $\mathbf{S}_0 = \text{const}$, and the equilibrium equation $\mathbf{L}^*(\nabla) \cdot \mathbf{T} = 0$ takes place for any given components of symmetric second rank stress tensor, then we have $\langle \mathbf{T} \cdot \mathbf{S} \rangle = \langle \mathbf{T} \rangle \cdot \langle \mathbf{S} \rangle$;

(b) $\varphi = -\mathbf{x} \cdot \mathbf{E}_0$, $\mathbf{E}_0 = \text{const}$, and the equation of electrostatics $\nabla \cdot \mathbf{D} = 0$ takes place for any given electric flux density vector \mathbf{D} , then we have $\langle \mathbf{D} \cdot \mathbf{E} \rangle = \langle \mathbf{D} \rangle \cdot \langle \mathbf{E} \rangle$;

(c) $\phi = -\mathbf{x} \cdot \mathbf{H}_0$, $\mathbf{H}_0 = \text{const}$, and the equation of magnetostatics $\nabla \cdot \mathbf{B} = 0$ takes place for any given magnetic flux density vector \mathbf{B} , then we have $\langle \mathbf{B} \cdot \mathbf{H} \rangle = \langle \mathbf{B} \rangle \cdot \langle \mathbf{H} \rangle$.

In accordance with fundamental form of constitutive equations we will introduce the moduli of the magnetoelectric medium (Eqs. (2)–(4) without damping effects):

$$\mathbf{T} = \mathbf{c} \cdot \mathbf{S} - \mathbf{e}^* \cdot \mathbf{E} - \mathbf{h}^* \cdot \mathbf{H}, \quad (30)$$

$$\mathbf{D} = \mathbf{e} \cdot \mathbf{S} + \boldsymbol{\kappa} \cdot \mathbf{E} + \boldsymbol{\alpha} \cdot \mathbf{H}, \quad (31)$$

$$\mathbf{B} = \mathbf{h} \cdot \mathbf{S} + \boldsymbol{\alpha}^* \cdot \mathbf{E} + \boldsymbol{\mu} \cdot \mathbf{H}. \quad (32)$$

For inhomogeneous two-phase magnetoelectric body these moduli will be functions of coordinates \mathbf{x} : $\mathbf{c} = \mathbf{c}(\mathbf{x})$; $\mathbf{e} = \mathbf{e}(\mathbf{x})$ etc., and $\boldsymbol{\alpha} = 0, \forall \mathbf{x} \in \Omega$; $\mathbf{q} = 0, \forall \mathbf{x} \in \Omega_e$; $\mathbf{e} = 0, \forall \mathbf{x} \in \Omega_m$.

Note that for the case of the piezoelectric medium we do not take into account the magnetic fields \mathbf{H} , \mathbf{B} , and we use the reduced constitutive equations

$$\mathbf{T} = \mathbf{c} \cdot \mathbf{S} - \mathbf{e}^* \cdot \mathbf{E},$$

$$\mathbf{D} = \mathbf{e} \cdot \mathbf{S} + \boldsymbol{\kappa} \cdot \mathbf{E}.$$

Let Ω be the representative volume of the heterogeneous magnetoelectric materials with piezoelectric and piezomagnetic phases. We will determine the effective moduli $\tilde{\mathbf{c}}, \tilde{\mathbf{e}}, \tilde{\mathbf{h}}, \tilde{\boldsymbol{\kappa}}, \tilde{\boldsymbol{\alpha}}, \tilde{\boldsymbol{\mu}}$ by the following technique, similar to the well-known procedures for purely elastic and piezoelectric composites [20, 24]. We consider the static magnetoelectric (piezomagnetoelectric or magnetoelectroelastic) problem for representative volume Ω :

$$\mathbf{L}^*(\nabla) \cdot \mathbf{T} = 0, \quad \nabla \cdot \mathbf{D} = 0, \quad \nabla \cdot \mathbf{B} = 0, \quad \mathbf{x} \in \Omega, \quad (33)$$

$$\mathbf{u} = \mathbf{L}^*(\mathbf{x}) \cdot \mathbf{S}_0, \quad \varphi = -\mathbf{x} \cdot \mathbf{E}_0, \quad \phi = -\mathbf{x} \cdot \mathbf{H}_0, \quad \mathbf{x} \in \Gamma. \quad (34)$$

From the solution of the problem (33), (34) and (5), (30)–(32) we find the fields \mathbf{S} , \mathbf{E} , \mathbf{H} , \mathbf{T} , \mathbf{D} and \mathbf{B} . We note from Lemma 2, that for the problem (5), (30)–(34): $\langle \mathbf{S} \rangle = \mathbf{S}_0$, $\langle \mathbf{E} \rangle = \mathbf{E}_0$ and $\langle \mathbf{H} \rangle = \mathbf{H}_0$.

Let us put some "equivalent" homogeneous medium with the effective moduli $\tilde{\mathbf{c}}, \tilde{\mathbf{e}}, \tilde{\mathbf{h}}, \tilde{\boldsymbol{\kappa}}, \tilde{\boldsymbol{\alpha}}, \tilde{\boldsymbol{\mu}}$ into correspondence with initial heterogeneous medium. The constitutive equations for "equivalent" medium, similar to (30)–(32), are given in the forms:

$$\mathbf{T}_0 = \tilde{\mathbf{c}} \cdot \mathbf{S}_0 - \tilde{\mathbf{e}}^* \cdot \mathbf{E}_0 - \tilde{\mathbf{h}}^* \cdot \mathbf{H}_0, \quad (35)$$

$$\mathbf{D}_0 = \tilde{\mathbf{e}} \cdot \mathbf{S}_0 + \tilde{\boldsymbol{\kappa}} \cdot \mathbf{E}_0 + \tilde{\boldsymbol{\alpha}} \cdot \mathbf{H}_0, \quad (36)$$

$$\mathbf{B}_0 = \tilde{\mathbf{h}} \cdot \mathbf{S}_0 + \tilde{\boldsymbol{\alpha}}^* \cdot \mathbf{E}_0 + \tilde{\boldsymbol{\mu}} \cdot \mathbf{H}_0. \quad (37)$$

For the problem (5), (30)–(34) we accept the following equations such as relations for determination of effective moduli from (35)–(37):

$$\langle \mathbf{T} \rangle = \mathbf{T}_0, \quad \langle \mathbf{D} \rangle = \mathbf{D}_0, \quad \langle \mathbf{B} \rangle = \mathbf{B}_0. \quad (38)$$

Note that due to Lemma 3 the average energies are equal for both heterogeneous and "equivalent" homogeneous magnetoelectric media:

$$\langle \mathbf{T} \cdot \mathbf{S} + \mathbf{D} \cdot \mathbf{E} + \mathbf{B} \cdot \mathbf{H} \rangle / 2 = (\mathbf{T}_0 \cdot \mathbf{S}_0 + \mathbf{D}_0 \cdot \mathbf{E}_0 + \mathbf{B}_0 \cdot \mathbf{H}_0) / 2.$$

Now, by using Eqs. (35)–(38), we can select such boundary conditions, that enable to obtain obvious expressions for the effective moduli. For example, we consider the problem (5), (30)–(34) with

$$S_{0\beta} = \varepsilon_0, \quad S_{0\gamma} = 0, \quad \gamma \neq \beta, \quad \mathbf{E}_0 = 0, \quad \mathbf{H}_0 = 0, \quad (39)$$

where β is some fixed number ($\beta = 1, 2, \dots, 6$); $\varepsilon_0 = \text{const}$. Then, from Eqs. (35)–(39) we obtain ($\alpha = 1, 2, \dots, 6$, $j = 1, 2, 3$):

$$\tilde{c}_{\alpha\beta} = \langle T_\alpha \rangle / (\varepsilon_0), \quad \tilde{e}_{j\beta} = \langle D_j \rangle / (\varepsilon_0), \quad \tilde{h}_{j\beta} = \langle B_j \rangle / (\varepsilon_0). \quad (40)$$

If in Eq. (34) we accept ($E_0 = \text{const}$)

$$\mathbf{S}_0 = 0, \quad \mathbf{E}_0 = E_0 \mathbf{e}_k, \quad \mathbf{H}_0 = 0, \quad (41)$$

where \mathbf{e}_k are the unit vectors of Cartesian basis, then from (35)–(38), (41) we find

$$\tilde{e}_{k\alpha} = -\langle T_\alpha \rangle / E_0, \quad \tilde{\kappa}_{jk} = \langle D_j \rangle / E_0, \quad \tilde{\alpha}_{kj} = \langle B_j \rangle / E_0. \quad (42)$$

Finally, if in Eq. (34) we accept ($H_0 = \text{const}$)

$$\mathbf{S}_0 = 0, \quad \mathbf{E}_0 = 0, \quad \mathbf{H}_0 = H_0 \mathbf{e}_k, \quad (43)$$

then from (35)–(38), (43) we find

$$\tilde{h}_{k\alpha} = -\langle T_\alpha \rangle / H_0, \quad \tilde{\alpha}_{jk} = \langle D_j \rangle / H_0, \quad \tilde{\mu}_{jk} = \langle B_j \rangle / H_0. \quad (44)$$

Note, that the quantities T_α , D_j and B_j in (40), (42) and (44) are different, since they are calculated from the solutions of the problems (5), (30)–(34) with various values \mathbf{S}_0 , \mathbf{E}_0 and \mathbf{H}_0 in the boundary conditions (34): (39), (41) and (43), respectively.

Equations (29), (39)–(44) allow us to obtain the full set of the effective moduli for magnetoelectric composite media with arbitrary anisotropy class. In this connection we can consider piezoelectric composite medium as a special case of magnetoelectric composite, where Ω_m is the empty set and $\Omega = \Omega_e$ is the region occupied by a heterogeneous body with only piezoelectric properties.

5 MODELLING OF THE REPRESENTATIVE VOLUMES AND FINITE ELEMENT SOLUTION

The use of the formulas presented above for the computation of the effective moduli leads to the solution of the corresponding boundary-value magnetoelectric problems in the regions Ω , that should be the representative volumes of the composite materials. Ideally, in order to be chosen as the representative volumes, the regions should be large enough compared to the sizes of the inhomogeneity but small enough compared to the distances where the slow variables considerably change.

Let us consider a binary composite, the first phase of which is the coherent structural skeleton from piezoelectric material and the second phase of which consists of isolated or connected with each other inclusions from piezomagnetic material. The first case according to the classification of R.E. Newnam corresponds to 3-0 connectivity and the second case corresponds to 3-3 connectivity (closed and open inclusions from piezomagnetic material, respectively).

Whereas the percentage of the entry of the second phase is relatively small, the model of cubic lattice appears to be rather simple but at the same time adequate representation of the microstructure for such composite material. The lattice consists of identical cells, or cubes, and some of these cubes are chosen at random to constitute the material of the second phase. We would like to note that such model does not support the structure of the composite connectivity (3-0 or 3-3).

For 3-0 and 3-3 connectivity types we use the special model built by the following manner [20]. The cube constructed by translation of identical solid cells along three directions is considered as a representative volume. Each cell in its turn also represents a cube consisting of $10 \times 10 \times 10$ cubic piezoelectric or piezomagnetic finite elements with 8 nodes each. A connected skeleton with piezoelectric finite elements in the cube corners always exists in the cell. The skeleton consists of a parallelepiped represented by its edges (linear dimensions are pointed out by the randomizer) as well as of piezoelectric elements chains connecting the corners of the parallelepiped with the corners of the main cell. The connecting piezoelectric finite elements chains are also generated by the randomizer. The skeleton occupies 10 % of the cell volume. So, the maximum possible porosity that can be achieved in this model runs up to 90 %. The representative volumes with large number of elements can be obtained by repetition of procedures for creating cubic structures of $10 \times 10 \times 10$ size along the three axes. In this case each structure of $10 \times 10 \times 10$ size is generated randomly in the frameworks of the procedures considered above. Additionally, in order to ensure smaller entrance of piezomagnetic material (up to zero) we have applied the following algorithm. Two cells are chosen randomly in the representative volume constructed at the previous step. If at least one of these cells is not a piezomagnetic material, then these cells are being linked by some arbitrary connected path. The resulting set is then added to the previously built frame consisting of solid piezoelectric elements. After that we calculate the current entrance of piezomagnetic material and compare it to the given entrance. If the calculated entrance of piezomagnetic material is less than the given entrance, the step of the algorithm should be repeated, i.e. again two cells should be randomly chosen in the representative volume, and so on.

In order to build connected structures in the cubic lattice it is possible also to use special algorithms and the algorithms of the percolation theory that allow obtaining flowing clusters. A range of such methods (random method, the initial concentration method, the DLA (diffusion-limited aggregation) method, Witten-Sander method, the DLA "growth from the plane" method, etc.) was implemented in the computer programs and analyzed in [20, 21] in relation to porous piezocomposite materials. For solving static piezomagnetolectric problems (33), (34) with (5), (30)–(32) for heterogeneous two-phase composite material in the representative volume Ω we can use the finite element technique, described in Sect. 3.

6 CONCLUSIONS

Thus, we have proposed an original model that describes the behavior of the magnetoelectric material, taking into account the damping properties and surface effects at the nanoscale level. Magnetoelectric material here is understood as a composite consisting of piezoelectric and piezomagnetic phases, and is used to describe the theory of coupled piezomagnetolectric medium with effective properties. In the particular case, when we neglect the coupling with magnetic fields, this model describes the behavior of a well-known piezoelectric material with damping properties and nanoscale effects.

We consider dynamic problems in quasistatic approximation for the electric and magnetic fields. The novelty of the model consists in taking into account the damping properties, as well as surface phenomena which are important

at the nanoscale.

To describe the size effects, we use recently popular theory of surface stresses and its generalization to piezomagneto-electric media. Under this generalization, we also consider the surface electric and magnetic fields.

Another 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 electric and magnetic fields. We also added the terms, describing the attenuation, in the constitutive equations for the surface mechanic, electric and magnetic fields. When taking the damping into account, the basic idea was that for some relation between the damping coefficients the method of mode superposition can be applied for transient and harmonic problems.

Examples of the finite element calculations for the case of piezoelectric bodies with surface effects previously appeared in [17, 19]. For calculations of magnetoelectric bodies, the developed technology can be extended within the same type of approaches. However, nowadays these approaches can not be used in practice, as there is not enough experimental data on the surface properties of nanosized magnetoelectric bodies.

We also developed the theory of the effective moduli method for magnetoelectric composites with piezoelectric and piezomagnetic phases. The basic statements were formulated for the average field characteristics that generalize the approaches developed for the elastic and piezoelectric media. The special boundary electromagnetoelastic problems for representative volume and necessary equations for the determination of the full set of the effective moduli were obtained for magnetoelectric media with arbitrary anisotropy.

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