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LOCAL GRADIENT THEORY FOR THERMOELASTIC DIELECTRICS: ACCOUNTING FOR MASS AND ELECTRIC CHARGE TRANSFER DUE TO MICROSTRUCTURE CHANGES

OLHA HRYTSYNA AND VASYL KONDRAT

In this paper a complete set of nonlinear field equations of a gradient-type continuum theory for thermoelastic nonferromagnetic dielectrics is obtained. The specification of the mentioned set of equations is based on the application of electrothermomechanical balance laws and takes into consideration the polarization electric current and mass flux (of nondiffusive and nonconvective nature) associated with microstructure changes. The electric current is caused by a change of both dipole and quadrupole electric moments over time, whilst the mass flux is caused by a change of the vector of the local mass displacement over time. The obtained set of equations accounts for the electromechanical coupling for isotropic materials and describes the near-surface, size, flexoelectric and thermopolarization effects. The classical theory of piezoelectrics is incapable of describing the mentioned phenomena. For isothermal linear approximation, the proposed theory is used to investigate the effect of thin-film thickness as well as of the diameter and surface curvature of a thin fiber and a cylindrical hole in elastic dielectrics on their stationary stress-strain state, bound surface electric charge, surface energy of deformation and polarization, etc. It is shown that a disjoining pressure emerges in thin films. This pressure can affect the strength and stability of nanoscale dielectric films. The results obtained in this paper are general and can be used for designing new nanocomposite materials and devices utilizing the micro/nanoscale films, fibers, etc.

A list of symbols including the notations used in this paper can be found on page 566. In general, bold symbols stand for vector quantities and bold symbols with caps denote second-order tensor quantities.

1. Introduction

The generalized theories of dielectrics have attracted the attention of many investigators. Extension of the classical field theory was stimulated by intensive development of new technologies, in particular, nanotechnologies, as well as by the availability of a number of inconsistencies in classical (local) theories. For example, classical theories predict a singular solution in problems with concentrated sources, cracks, and defects. Some experimental results (namely, polarization of a material with centrosymmetry under nonuniform mechanical loads or temperature gradients [Kholkin et al. 1982; Zholudev 1966], nonlinear dependence of capacitance of thin dielectric film on its thickness, known as Mead's anomaly [Mead 1961], size effects [Axe et al. 1970; Nam et al. 2006; Tang and Alici 2011] etc.) are outside the scope of classical theories of dielectrics.

There are several different ways of constructing extended theories of elastic dielectrics. One group of theories considers the additional degrees of freedom (i.e., microrotations, microdeformations, etc.) for

Keywords: local gradient theory, electric quadrupole moment, local mass displacement, surface and size effects.

material points in order to model the contribution of the microstructure changes to the macroscopic behavior of the body. In such a way there were developed more general theories, in particular, micromorphic, microstretch, micropolar continua, etc. [Eringen 1966; 1999; Eringen and Suhubi 1964]. The nonlocal and gradient theories form another group of extended theories of dielectrics. The nonlocal field theory for piezoelectricity with functional constitutive relations was proposed in [Eringen 1984; 2002]. The gradient-type theories were mainly formulated using the variation methods or methods of nonequilibrium thermodynamics [Kalpakidis and Massalas 1993; Maugin 1980; Nowacki 1983; Papenfuss and Forest 2006; Ván 2003]. Such theories were developed by allowing the stored energy density to depend on the gradient of some physical quantities, namely, the strain tensor gradient [Mindlin 1965], the polarization gradient [Mindlin 1968], or the electric field gradient [Kafadar 1971; Kalpakides and Agiasofitou 2002; Kalpakidis and Massalas 1993; Maugin 1988]. Note that the electric field gradient is a thermodynamic conjugate of the electric quadrupole [Kafadar 1971]. For a more detailed description of these theories, see monographs [Burak et al. 2011; Eringen 1999; 2002; Erofeyev 2003; Maugin 1988; Nowacki 1983; 1986] and reviews [Kondrat and Hrytsyna 2009; Yang 2006].

Burak et al. [2007; 2008] proposed a continuum-thermodynamical approach to the construction of a gradient-type theory of electrothermoelasticity of polarized solids (local gradient electrothermomechanics of dielectrics, in the author's terminology). The mentioned approach is based on accounting for nondiffusive and nonconvective mass fluxes associated with changes in the material microstructure. These fluxes are related to the process of local mass displacement [Burak et al. 2007; 2008].

The objective of this paper is to develop this approach and to construct the local gradient theory of nonferromagnetic dielectrics that accounts for the above mass fluxes as well as for the polarization currents. Here, we will consider the contribution of electric dipole and quadrupole moments to the polarization current. The developed theory will be used for describing near-surface and size effects, in particular, to investigate the surface energy of deformation and polarization, a disjoining pressure in thin solid films, etc.

2. Investigation object and notations

We consider an electrically polarizable nonferromagnetic heat-conducting elastic body which occupies the domain (V_*) of three-dimensional Euclidean space with a smooth surface (Σ_*). In view of the action of external forces, electromagnetic field and heating of the body, mechanical, thermal, and electromagnetic processes can occur within the solid. These processes may be accompanied by changes in the microstructure of a small body element (dV) (representative volume). We characterize these changes by an electric flux $\boldsymbol{J}_{es}$ (polarization current) and a nonconvective and nondiffusive mass flux $\boldsymbol{J}_{ms}$. It should be noted that Marchenko et al. [2009] observed the mentioned nondiffusive mass flux within the near-surface domains of thin films during their formation. We relate the mass flux $\boldsymbol{J}_{ms}$ to the process of the local mass displacement [Burak et al. 2007; 2008].

All fields that characterize the processes occurring in the solid should obey the fundamental laws of continuum physics, namely, the Maxwell equations and the corresponding balance laws (balances of energy, mass, linear momentum, angular momentum, and entropy).

3. Conservation laws of mass and induced mass

We separate from the body a fixed small volume (V) bounded by closed surface (Σ). The interaction of the microparticles of the considered volume (V) with the exterior microparticles occurs through the surface (Σ). The integral form of the mass balance equation for the considered volume can be written as

$$\frac{d}{dt}\int_{(V)} \rho\, dV = -\oint_{(\Sigma)} \boldsymbol{J}_{m^*} \cdot \boldsymbol{n}\, d\Sigma. \tag{1}$$

Here, ρ is the mass density, $\boldsymbol{J}_{m^*}$ is the density of mass flux, $\boldsymbol{n}$ is the outward unit normal to the surface (Σ), and the dot denotes the scalar product.

We take into consideration that the mass-center displacement of the representative volume may be induced not only by its convective displacement as a rigid entity (i.e., translational displacement of the element geometric center) but also by the changes of the relative positions of microparticles within this element, that is, the change of its microstructure (see Figure 1). In view of this, we represent the mass flux $\boldsymbol{J}_{m^*}$ as the sum of the convective component $\rho\boldsymbol{v}_*$ and component $\boldsymbol{J}_{ms}$ related to the ordering of microstructure of the representative volume, that is $\boldsymbol{J}_{m^*} = \rho\boldsymbol{v}_* + \boldsymbol{J}_{ms}$. Here, $\boldsymbol{v}_* = \dot{\boldsymbol{u}}_*$ is the velocity vector of convective displacement of the representative volume, $\boldsymbol{u}_* = \boldsymbol{r}_* - \boldsymbol{r}_0$ (Figure 1). Hence, equation (1) in the local form can be written as

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\boldsymbol{v}_* + \boldsymbol{J}_{ms}) = 0, \tag{2}$$

where $\boldsymbol{\nabla}$ is the Hamilton operator.

We introduce the velocity vector $\boldsymbol{v}$ of the center of mass by the formula [Burak et al. 2007; 2008]

$$\boldsymbol{v} = \frac{1}{\rho}(\rho\boldsymbol{v}_* + \boldsymbol{J}_{ms}). \tag{3}$$

In view of formula (3), the equation of mass balance (2) can be written in the standard form

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\boldsymbol{v}) = 0. \tag{4}$$

Following Burak et al. [2007; 2008], assume that the mass flux $\boldsymbol{J}_{ms}$ is caused by a change over time of the mass dipole moment $\boldsymbol{\Pi}_m$ (i.e., the vector of local mass displacement):

$$\boldsymbol{J}_{ms} = \partial\boldsymbol{\Pi}_m/\partial t. \tag{5}$$

To describe the local mass displacement by the formula

$$\int_{(V_*)} \boldsymbol{\Pi}_m\, dV = \int_{(V_*)} \rho_{m\pi}\, \boldsymbol{r}\, dV, \tag{6}$$

we also introduce the density of induced mass $\rho_{m\pi}$ [Burak et al. 2008]. In (6), we integrate over the volume (V_*) of the solid body. Note that from the integral equation (6) the following useful relations can be easily obtained:

$$\int_{(V_*)} \rho_{m\pi}\, dV = 0, \tag{7}$$

$$\rho_{m\pi} = -\boldsymbol{\nabla}\cdot\boldsymbol{\Pi}_m. \tag{8}$$

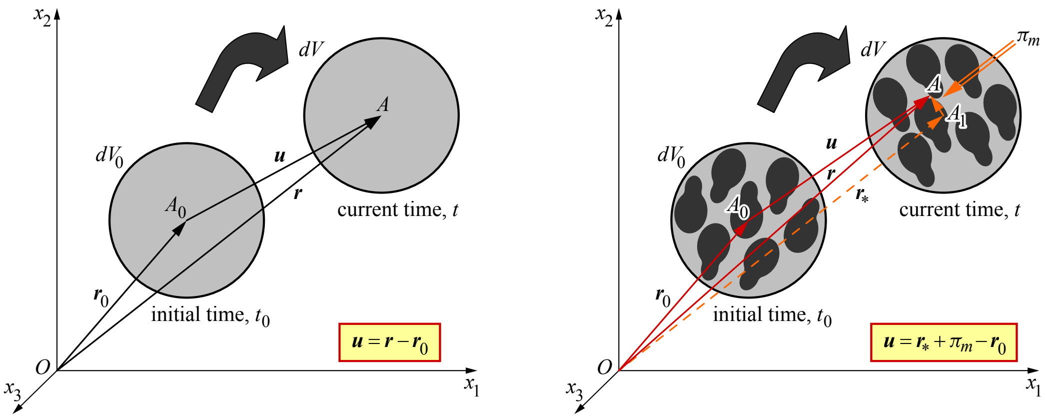

Figure 1. Changing the center of mass of a small body element within the classical theory ($\boldsymbol{u} = \boldsymbol{r} - \boldsymbol{r}_0$) (left), and local gradient theory taking the local mass displacement into account ($\boldsymbol{u} = \boldsymbol{r}_* + \pi_m - \boldsymbol{r}_0$, where $\pi_m = \Pi_m/\rho$) (right).

Let's derive the formula (8). To this end, we multiply the lefthand and righthand sides of the relation (6) by an arbitrary constant vector $\boldsymbol{a}$ and use the identity $\boldsymbol{a} \cdot \boldsymbol{\Pi}_m = (\boldsymbol{\Pi}_m \cdot \nabla)(\boldsymbol{a} \cdot \boldsymbol{r})$. As a result, after some algebra, we obtain

$$\int_{(V_*)} (\boldsymbol{a} \cdot \boldsymbol{r})\, \rho_{m\pi}\, dV = \int_{(V_*)} (\boldsymbol{\Pi}_m \cdot \nabla)(\boldsymbol{a} \cdot \boldsymbol{r})\, dV = -\int_{(V_*)} \nabla \cdot [\boldsymbol{\Pi}_m (\boldsymbol{a} \cdot \boldsymbol{r})]\, dV - \int_{(V_*)} (\boldsymbol{a} \cdot \boldsymbol{r})(\nabla \cdot \boldsymbol{\Pi}_m)\, dV. \quad (9)$$

Assume that the body comes in contact with vacuum. Since vector $\boldsymbol{\Pi}_m$ is equal to zero outside the body, then

$$\int_{(V_*)} \nabla \cdot [\boldsymbol{\Pi}_m (\boldsymbol{a} \cdot \boldsymbol{r})]\, dV = 0. \quad (10)$$

Because vector $\boldsymbol{a}$ is arbitrary, from the expression (9) we get formula (8). Similarly, formula (7) can be obtained [Burak et al. 2011].

By differentiating formula (8) with respect to time and taking relation (5) into account, one can obtain a conservation law of an induced mass:

$$\frac{\partial \rho_{m\pi}}{\partial t} + \nabla \cdot \boldsymbol{J}_{ms} = 0. \quad (11)$$

4. Electrodynamics equations

The Maxwell equations in the local form are given by [Landau and Lifshitz 1982]

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}, \quad \nabla \times \boldsymbol{H} = \boldsymbol{J}_{ef}, \quad (12)$$

$$\nabla \cdot \boldsymbol{B} = 0, \quad \nabla \cdot \boldsymbol{D} = \rho_e. \quad (13)$$

Here $\boldsymbol{J}_{ef} = \boldsymbol{J}_e + \boldsymbol{J}_{ed} + \boldsymbol{J}_{es}$, where $\boldsymbol{J}_e$ is the density of the electric current (convection and conduction currents), $\boldsymbol{J}_{es}$ is the polarization current, and $\boldsymbol{J}_{ed} = \varepsilon_0(\partial \boldsymbol{E}/\partial t)$, ε_0 is the electric permittivity of a vacuum.

Assume that the polarization current $\boldsymbol{J}_{es}$ is caused by a change over time of both the dipole $\boldsymbol{P}$ and the quadrupole $\hat{\boldsymbol{Q}}$ electric moments [Kondrat and Hrytsyna 2019], namely

$$\boldsymbol{J}_{es} = \frac{\partial \boldsymbol{\Pi}_e}{\partial t}, \quad \boldsymbol{\Pi}_e = \boldsymbol{P} - \frac{1}{6}\nabla \cdot \hat{\boldsymbol{Q}}. \tag{14}$$

Here, $\boldsymbol{\Pi}_e$ is the polarization vector, which can be thought of as a vector of the local displacement of electric charges. Thus, using (14), one can write

$$\boldsymbol{J}_{ef} = \boldsymbol{J}_e + \varepsilon_0 \frac{\partial \boldsymbol{E}}{\partial t} + \frac{\partial \boldsymbol{\Pi}_e}{\partial t}. \tag{15}$$

For nonferromagnetic dielectrics, the constitutive equations for the vectors of magnetic $\boldsymbol{B}$ and electric $\boldsymbol{D}$ inductions look like

$$\boldsymbol{B} = \mu_0 \boldsymbol{H}, \quad \boldsymbol{D} = \varepsilon_0 \boldsymbol{E} + \boldsymbol{P} - \frac{1}{6}\nabla \cdot \hat{\boldsymbol{Q}}. \tag{16}$$

Here, μ_0 is the magnetic permeability in vacuum. We also introduce the density of an induced charge $\rho_{e\pi}$ [Bredov et al. 1985]

$$\int_{(V_*)} \boldsymbol{\Pi}_e \, dV = \int_{(V_*)} \rho_{e\pi} \boldsymbol{r} \, dV. \tag{17}$$

From (17) it follows that [Bredov et al. 1985]

$$\int_{(V_*)} \rho_{e\pi} \, dV = 0, \quad \rho_{e\pi} = -\nabla \cdot \boldsymbol{\Pi}_e. \tag{18}$$

The conservation law of induced electric charges looks like [Bredov et al. 1985]

$$\frac{\partial \rho_{e\pi}}{\partial t} + \nabla \cdot \boldsymbol{J}_{es} = 0. \tag{19}$$

Equations (12), (13), (15), and (16) yield the following balance law for the energy U_e of the electromagnetic field [Burak et al. 2011]:

$$\frac{\partial U_e}{\partial t} + \nabla \cdot \boldsymbol{S}_e + \left(\boldsymbol{J}_e + \frac{\partial \boldsymbol{\Pi}_e}{\partial t} \right) \cdot \boldsymbol{E} = 0. \tag{20}$$

Here, $U_e = (\varepsilon_0 \boldsymbol{E}^2 + \mu_0^{-1} \boldsymbol{B}^2)/2$, $\boldsymbol{S}_e = \mu_0^{-1} \boldsymbol{E} \times \boldsymbol{B}$. Note that the last term in (20) describes the effect of the electromagnetic field on a substance. Let us rewrite the above term in such a way that it contains the quadrupole $\hat{\boldsymbol{Q}}_*$ and dipole $\boldsymbol{P}_*$ electric moments, the electric field vector $\boldsymbol{E}_*$, and the density of the electric current $\boldsymbol{J}_{e^*}$ in the reference frame of the mass centers moving with a velocity $\boldsymbol{v}$ relative to the laboratory reference frame. In this co-moving frame, the vectors $\boldsymbol{E}$, $\boldsymbol{P}$, $\boldsymbol{J}_e$ and the tensor $\hat{\boldsymbol{Q}}$ are transformed according to the relations: $\boldsymbol{E} = \boldsymbol{E}_* - \boldsymbol{v} \times \boldsymbol{B}$, $\boldsymbol{P} = \boldsymbol{P}_*$, $\boldsymbol{J}_e = \boldsymbol{J}_{e^*} + \rho_e \boldsymbol{v}$, $\hat{\boldsymbol{Q}} = \hat{\boldsymbol{Q}}_*$. Here, the vector $\boldsymbol{J}_{e^*}$ is the conduction current density. Substituting these equations into (20) and using the mass conservation law (4), the balance equation for the energy of the electromagnetic field can be reduced to the following form:

$$\frac{\partial U_e}{\partial t}+\nabla\cdot\boldsymbol{S_e}+\boldsymbol{J}_{e^*}\cdot\boldsymbol{E}_*+\rho\frac{D\boldsymbol{p}}{Dt}\cdot\boldsymbol{E}_*+\rho\frac{D\hat{\boldsymbol{q}}}{Dt}:(\nabla\otimes\boldsymbol{E}_*)$$
$$+\boldsymbol{v}\cdot\left[\rho_e\boldsymbol{E}_*+\left(\boldsymbol{J}_{e^*}+\frac{\partial\boldsymbol{\Pi}_e}{\partial t}\right)\times\boldsymbol{B}+\rho(\nabla\otimes\boldsymbol{E}_*)\cdot\boldsymbol{p}-\rho(\nabla\otimes\nabla\otimes\boldsymbol{E}_*):\hat{\boldsymbol{q}}\right]$$
$$-\nabla\cdot\{[\boldsymbol{p}\cdot\boldsymbol{E}_*+\hat{\boldsymbol{q}}:(\nabla\otimes\boldsymbol{E}_*)]\rho\boldsymbol{v}\}=0. \quad (21)$$

Here, $\boldsymbol{p}=\boldsymbol{P}/\rho$ and $\hat{\boldsymbol{q}}=\hat{\boldsymbol{Q}}/6\rho$, $\otimes$ is the tensor product, and $\frac{D\ldots}{Dt}=\frac{\partial\ldots}{\partial t}+\boldsymbol{v}\cdot\nabla\ldots$ denotes the material time derivative.

5. Equation of entropy balance

We used the approaches of classical nonequilibrium thermodynamics. Within the nonequilibrium thermodynamics, the entropy balance equation may be expressed in the local form as [de Groot and Mazur 1962]

$$\rho\frac{Ds}{Dt}=-\nabla\cdot\left(\frac{\boldsymbol{J}_q}{T}\right)+\eta+\rho\frac{\mathfrak{R}}{T}. \quad (22)$$

Here, s is the specific entropy, $\boldsymbol{J}_q$ is the density of the heat flux, T is the absolute temperature, $\mathfrak{R}$ denotes the distributed heat source, and η is the entropy production per unit of volume and time.

6. Energy balance law for system "solid-electromagnetic field"

We assume that the total energy $\mathscr{E}$ is the sum of internal energy ρu (u is the specific internal energy), kinetic energy $\rho\boldsymbol{v}^2/2$, and the energy U_e of the electromagnetic field: $\mathscr{E}=\rho u+\frac{1}{2}\rho\boldsymbol{v}^2+U_e$. We also assume that the change in the total energy is caused (i) by the convective energy transport $\rho(u+\boldsymbol{v}^2/2)$ through the body surface, (ii) by the energy flux $\hat{\sigma}\cdot\boldsymbol{v}$ due to the power of surface forces, (iii) by the heat flux $\boldsymbol{J}_q$, (iv) by the electromagnetic energy flux $\boldsymbol{S}_e$, (v) by the energy flux $\mu\boldsymbol{J}_m$ linked with the mass transport relative to the centre of mass of the small body element, (vi) by the energy flux $\mu_\pi\boldsymbol{J}_{ms}$ related to the material microstructure ordering (i.e., local mass displacement), as well as (vii) by the action of mass forces $\boldsymbol{F}$ and (viii) by the action of distributed heat sources $\mathfrak{R}$. Thus, the law of the energy balance can be written as

$$\frac{d}{dt}\int_{(V)}\mathscr{E}\,dV=-\oint_{(\Sigma)}\left[\rho\left(u+\frac{1}{2}\boldsymbol{v}^2\right)\boldsymbol{v}-\hat{\sigma}\cdot\boldsymbol{v}+\boldsymbol{S}_e+\boldsymbol{J}_q+\mu\boldsymbol{J}_m+\mu_\pi\boldsymbol{J}_{ms}\right]\cdot\boldsymbol{n}\,d\Sigma+\int_{(V)}(\rho\boldsymbol{F}\cdot\boldsymbol{v}+\rho\mathfrak{R})\,dV, \quad (23)$$

where $\hat{\sigma}$ is the Cauchy stress tensor, μ is chemical potential, μ_π is an energy measure of the effect of the local mass displacement on the internal energy and $\boldsymbol{J}_m=\rho(\boldsymbol{v}_*-\boldsymbol{v})$ [Burak et al. 2008].

By the use of (4), (5), (8), (21), and (22), taking a time derivative of the righthand side of (23) and by means of the divergence theorem, after some lengthy algebraic manipulations, we obtain the following local form of the balance equation for the internal energy u:

$$\rho\frac{Du}{Dt}=\rho T\frac{Ds}{Dt}+\hat{\sigma}_*:\frac{D\hat{\boldsymbol{e}}}{Dt}+\rho\boldsymbol{E}_*\cdot\frac{D\boldsymbol{p}}{Dt}+\rho\nabla\otimes\boldsymbol{E}_*:\frac{D\hat{\boldsymbol{q}}}{Dt}+\rho\mu'_\pi\frac{D\rho_m}{Dt}-\rho\nabla\mu'_\pi\cdot\frac{D\boldsymbol{\pi}_m}{Dt}$$
$$+\boldsymbol{J}_{e^*}\cdot\boldsymbol{E}_*-\boldsymbol{J}_q\cdot\frac{\nabla T}{T}-T\eta+\boldsymbol{v}\cdot\left[-\rho\frac{D\boldsymbol{v}}{Dt}+\nabla\cdot\hat{\sigma}_*+\boldsymbol{F}_e+\rho(\boldsymbol{F}+\boldsymbol{F}_m)\right], \quad (24)$$

where $\boldsymbol{\pi}_m = \boldsymbol{\Pi}_m/\rho$; $\rho_m = \rho_{m\pi}/\rho$; $\mu'_\pi = \mu_\pi - \mu$. Here, $\hat{\boldsymbol{e}}$, $\boldsymbol{F}_e$, $\boldsymbol{F}_m$, and $\hat{\sigma}_*$ are the infinitesimal strain tensor, ponderomotive force, additional mass force, and modified stress tensor that are defined by

$$\hat{\boldsymbol{e}} = [\nabla \otimes \boldsymbol{u} + (\nabla \otimes \boldsymbol{u})^T]/2, \tag{25}$$

$$\boldsymbol{F}_e = \rho_e \boldsymbol{E}_* + \rho(\nabla \otimes \boldsymbol{E}_*) \cdot \boldsymbol{p} + \left(\boldsymbol{J}_{e^*} + \frac{\partial \boldsymbol{\Pi}_e}{\partial t} \right) \times \boldsymbol{B} + \rho(\nabla \otimes \nabla \otimes \boldsymbol{E}_*)^{T(2,3)} : \hat{\boldsymbol{q}}, \tag{26}$$

$$\boldsymbol{F}_m = \rho_m \nabla \mu'_\pi - (\nabla \otimes \nabla \mu'_\pi) \cdot \boldsymbol{\pi}_m, \tag{27}$$

$$\hat{\sigma}_* = \hat{\sigma} - \rho[\boldsymbol{p} \cdot \boldsymbol{E}_* + \hat{\boldsymbol{q}} : (\nabla \otimes \boldsymbol{E}_*) + \rho_m \mu'_\pi - \boldsymbol{\pi}_m \cdot \nabla \mu'_\pi]\hat{\boldsymbol{I}}, \tag{28}$$

where superscript $\langle T \rangle$ denotes a transposed tensor and $\hat{\boldsymbol{I}}$ is the unit tensor.

Applying the principle of frame indifference in a rigid translation, from (21) we obtain the balance of momentum in the form

$$\rho(D\boldsymbol{v}/Dt) = \nabla \cdot \hat{\sigma}_* + \boldsymbol{F}_e + \rho(\boldsymbol{F} + \boldsymbol{F}_m). \tag{29}$$

It is evident from (29), that the electric quadrupole and mass dipole moments induce nonlinear body forces $\boldsymbol{F}'_e = -\rho(\nabla \otimes \nabla \otimes \boldsymbol{E}_*) : \hat{\boldsymbol{q}}$ and $\boldsymbol{F}_m$ and couple stresses $\hat{\sigma}'_* = -\rho[\hat{\boldsymbol{q}} : (\nabla \otimes \boldsymbol{E}_*) + \rho_m \mu'_\pi - \boldsymbol{\pi}_m \cdot \nabla \mu'_\pi]\hat{\boldsymbol{I}}$ within the body. Note that as evident from relation (25), we confined ourselves to linear strain-displacement relations (i.e., geometric nonlinearity is neglected within the framework of constructed mathematical model) whereas the balance equations (4), (11), (22), and (29) are nonlinear (the model takes physical nonlinearity into account).

By means of the Legendre transformation $f = u - Ts - \boldsymbol{E}_* \cdot \boldsymbol{p} - \hat{\boldsymbol{q}} : (\nabla \otimes \boldsymbol{E}_*) + \nabla \mu'_\pi \cdot \boldsymbol{\pi}_m$ we define the generalized Helmholtz free energy. Using this new thermodynamic function and the balance of linear momentum (29), from (24) we obtain

$$\rho \frac{Df}{Dt} = -\rho s \frac{DT}{Dt} + \hat{\sigma}_* : \frac{D\hat{\boldsymbol{e}}}{Dt} - \rho \boldsymbol{p} \cdot \frac{D\boldsymbol{E}_*}{Dt} - \rho \hat{\boldsymbol{q}} : \frac{D(\nabla \otimes \boldsymbol{E}_*)}{Dt} + \rho \mu'_\pi \frac{D\rho_m}{Dt} + \rho \boldsymbol{\pi}_m \cdot \frac{D\nabla \mu'_\pi}{Dt} + \boldsymbol{J}_{e^*} \cdot \boldsymbol{E}_* - \boldsymbol{J}_q \cdot \frac{\nabla T}{T} - T\eta. \tag{30}$$

While inspecting (30), we assume that the Helmholtz free energy is a function of T, $\hat{\boldsymbol{e}}$, $\boldsymbol{E}_*$, $\nabla \otimes \boldsymbol{E}_*$, ρ_m, and $\nabla \mu'_\pi$ that is $f = f(T, \hat{\boldsymbol{e}}, \boldsymbol{E}_*, \nabla \otimes \boldsymbol{E}_*, \rho_m, \nabla \mu'_\pi)$. Note that the density of free energy depends not only on temperature T, strain tensor $\hat{\boldsymbol{e}}$, and electric field vector $\boldsymbol{E}_*$, as it follows from the classical theories, but also on the parameters $\nabla \otimes \boldsymbol{E}_*$, $\rho_m = -\nabla \cdot (\rho \boldsymbol{\pi}_m)/\rho$, and $\nabla \mu'_\pi$, related to the electric quadrupole and mass dipole moments. Using (30), we get the expression

$$\rho\left(\frac{\partial f}{\partial T} + s\right)\frac{DT}{Dt} + \left(\rho \frac{\partial f}{\partial \hat{\boldsymbol{e}}} - \hat{\sigma}_*\right) : \frac{D\hat{\boldsymbol{e}}}{Dt} + \rho\left(\frac{\partial f}{\partial \boldsymbol{E}_*} + \boldsymbol{p}\right) \cdot \frac{D\boldsymbol{E}_*}{Dt} + \rho\left(\frac{\partial f}{\partial(\nabla \otimes \boldsymbol{E}_*)} + \hat{\boldsymbol{q}}\right) : \frac{D(\nabla \otimes \boldsymbol{E}_*)}{Dt} + \rho\left(\frac{\partial f}{\partial \rho_m} - \mu'_\pi\right)\frac{D\rho_m}{Dt} + \rho\left(\frac{\partial f}{\partial \nabla \mu'_\pi} - \boldsymbol{\pi}_m\right) \cdot \frac{D\nabla \mu'_\pi}{Dt} = 0, \tag{31}$$

and the following relation for entropy production

$$\eta = \boldsymbol{J}_{e^*} \cdot \boldsymbol{E}_* - \boldsymbol{J}_q \cdot (\nabla T/T). \tag{32}$$

Note that in relation (32) for entropy production, the terms caused by polarization and the local mass displacement are absent because we describe these processes as reversible.

7. Constitutive equations

Since parameters T, $\hat{\boldsymbol{e}}$, $\boldsymbol{E}_*$, $\nabla\otimes\boldsymbol{E}_*$, ρ_m, and $\nabla\mu'_\pi$ are independent, we obtain the following constitutive equations from relation (31):

$$\hat{\sigma}_* = \rho\frac{\partial f}{\partial\hat{\boldsymbol{e}}}\bigg|_{T,\boldsymbol{E}_*,\nabla\otimes\boldsymbol{E}_*,\rho_m,\nabla\mu'_\pi}, \qquad s = -\frac{\partial f}{\partial T}\bigg|_{\hat{\boldsymbol{e}},\boldsymbol{E}_*,\nabla\otimes\boldsymbol{E}_*,\rho_m,\nabla\mu'_\pi}, \qquad \boldsymbol{p} = -\frac{\partial f}{\partial\boldsymbol{E}_*}\bigg|_{\hat{\boldsymbol{e}},T,\nabla\otimes\boldsymbol{E}_*,\rho_m,\nabla\mu'_\pi}, \tag{33}$$

$$\hat{\boldsymbol{q}} = -\frac{\partial f}{\partial(\nabla\otimes\boldsymbol{E}_*)}\bigg|_{\hat{\boldsymbol{e}},T,\boldsymbol{E}_*,\rho_m,\nabla\mu'_\pi}, \qquad \mu'_\pi = \frac{\partial f}{\partial\rho_m}\bigg|_{\hat{\boldsymbol{e}},T,\boldsymbol{E}_*,\nabla\otimes\boldsymbol{E}_*,\nabla\mu'_\pi}, \qquad \boldsymbol{\pi}_m = \frac{\partial f}{\partial(\nabla\mu'_\pi)}\bigg|_{\hat{\boldsymbol{e}},T,\boldsymbol{E}_*,\nabla\otimes\boldsymbol{E}_*,\rho_m}. \tag{34}$$

The specific electric quadrupole $\hat{\boldsymbol{q}}$, the potential μ'_π, and the local mass displacement vector $\boldsymbol{\pi}_m$ are the thermodynamic conjugates of the electric field gradient, the specific induced mass, and the gradient of modified chemical potential.

We can write (33) and (34) in an explicit form. In order to obtain the linear constitutive relations, we expand f into a Taylor series about $\hat{\boldsymbol{e}}=0$, $T=T_0$, $\boldsymbol{E}_*=0$, $\nabla\otimes\boldsymbol{E}_*=0$, $\rho_m=0$, $\mu'_\pi=\mu'_{\pi 0}$, and $\nabla\mu'_\pi=0$, where T_0 is a reference temperature and $\mu'_{\pi 0}$ is the potential μ'_π of an infinite medium. Denoting $\theta=T-T_0$, $I_{e1}=\hat{\boldsymbol{e}}:\hat{\boldsymbol{I}}=e$, $I_{e2}=\hat{\boldsymbol{e}}:\hat{\boldsymbol{e}}$, $I_{E1}=(\nabla\otimes\boldsymbol{E}_*):\hat{\boldsymbol{I}}=\nabla\otimes\boldsymbol{E}_*$, $I_{E2}=(\nabla\otimes\boldsymbol{E}_*):(\nabla\otimes\boldsymbol{E}_*)$ and keeping linear and quadratic terms only, we can write the following for isotropic materials

$$\begin{aligned} f = f_0 - s_0\theta + \mu'_{\pi 0}\rho_m + \frac{1}{2\rho_0}\left(K-\frac{2}{3}G\right)I_{e1}^2 + \frac{G}{\rho_0}I_{e2} - \frac{C_V}{2T_0}\theta^2 + \frac{d_\rho}{2}\rho_m^2 \\ - \frac{\chi_m}{2}(\nabla\mu'_\pi)^2 - \frac{\chi_E}{2}\boldsymbol{E}_*^2 + \frac{\chi_{q1}}{2}I_{E1}^2 - \chi_{q2}I_{E2} - \frac{K\alpha_T}{\rho_0}I_{e1}\theta - \frac{K\alpha_\rho}{\rho}I_{e1}\rho_m \\ - \frac{K\alpha_{E1}}{\rho_0}I_{e1}I_{E1} - \beta_{T\rho}\rho_m\theta + \beta_{TE}I_{E1}\theta + \beta_{E\rho}I_{E1}\rho_m \\ + \chi_{Em}\boldsymbol{E}_*\cdot\nabla\mu'_\pi + 2G\frac{\alpha_{E2}}{\rho_0}\hat{\boldsymbol{e}}:(\nabla\otimes\boldsymbol{E}_*). \end{aligned} \tag{35}$$

Here K, G, C_V, d_ρ, α_T, α_ρ, α_{E1}, α_{E2}, χ_E, χ_m, χ_{Em}, χ_{q1}, χ_{q2}, $\beta_{T\rho}$, β_{TE}, $\beta_{E\rho}$ are material characteristics.

Using the formulas (33), (34) and (35) we obtain the following constitutive relations for isotropic dielectric materials

$$\hat{\sigma} = 2G\hat{\boldsymbol{e}} + 2G\alpha_{E2}\nabla\otimes\boldsymbol{E} + \left[\left(K-\frac{2}{3}G\right)e - K\alpha_T\theta - K\alpha_\rho\rho_m - K\alpha_{E1}\nabla\cdot\boldsymbol{E}\right]\hat{\boldsymbol{I}}, \tag{36a}$$

$$s = s_0 + \frac{C_V}{T_0}\theta + \frac{K\alpha_T}{\rho_0}e + \beta_{T\rho}\rho_m - \beta_{TE}\nabla\cdot\boldsymbol{E}, \tag{36b}$$

$$\mu'_\pi = \mu'_{\pi 0} + d_\rho\rho_m - \frac{K\alpha_\rho}{\rho_0}e - \beta_{T\rho}\theta + \beta_{E\rho}\nabla\cdot\boldsymbol{E}, \tag{36c}$$

$$\boldsymbol{p} = \chi_E\boldsymbol{E} - \chi_{Em}\nabla\mu'_\pi, \tag{36d}$$

$$\boldsymbol{\pi}_m = -\chi_m\nabla\mu'_\pi + \chi_{Em}\boldsymbol{E}, \tag{36e}$$

$$\hat{\boldsymbol{q}} = 2\chi_{q2}\nabla\otimes\boldsymbol{E} - 2G\alpha_{E2}\hat{\boldsymbol{e}} - \left(\chi_{q1}\nabla\cdot\boldsymbol{E} - \frac{K\alpha_{E1}}{\rho_0}e + \beta_{TE}\theta + \beta_{E\rho}\rho_m\right)\hat{\boldsymbol{I}}. \tag{36f}$$

The constitutive equations describe an electromechanical interaction in isotropic (centrosymmetric) materials. In the framework of the proposed theory, the body polarization is caused not only by the electric field but also by the spatial nonhomogeneity of the field, as well as by the gradients of the strain, and the temperature and density of induced mass. Hence, the constitutive equations (36) for isotropic materials make it possible to describe both the flexoelectric and thermopolarization effects. Note that the classical theories of dielectrics cannot describe these effects.

Now we shall specify the expressions for fluxes. We represent (32) for entropy production as follows: $\eta = \frac{1}{T}\sum_{k=1}^{2} \boldsymbol{j}_k \cdot \boldsymbol{X}_k$, where $\boldsymbol{J}_1 = \boldsymbol{J}_{e^*}$, $\boldsymbol{J}_2 = \boldsymbol{J}_q$, $\boldsymbol{X}_1 = \boldsymbol{E}_*$, and $\boldsymbol{X}_2 = -\nabla T/T$ are thermodynamic fluxes and forces. Assuming that thermodynamic forces are the cause of the thermodynamic fluxes $\boldsymbol{j}_1$ and $\boldsymbol{j}_2$, we can write $\boldsymbol{j}_i = \boldsymbol{j}_i(\boldsymbol{X}_1, \boldsymbol{X}_2),\ i = 1, 2$. In a linear approximation, we obtain the following equations for fluxes

$$\boldsymbol{J}_e = \zeta_E \boldsymbol{E} - \zeta \nabla T, \qquad \boldsymbol{J}_q = -\lambda \nabla T + \zeta_T \boldsymbol{J}_e, \tag{37}$$

where ζ_E and λ are electric and thermal conductivity, respectively, and the coefficients ζ_T and ζ characterize thermoelectric phenomena. Note that the Second Law of thermodynamics states that entropy production is positive definite, i.e., $\eta \geq 0$. In order to ensure the positive character of entropy production, the coefficients λ, ζ_E, ζ, and ζ_T should be positive defined.

8. Key equations for isothermal approximation

Balance equations (11), (19), (22), (29), Maxwell's equations (12), (13), constitutive relations (16), (36), (37), and formulas (5), (14), (15), (25) form a complete set of field equations for the coupled problems of local gradient electrothermoelasticity for nonferromagnetic dielectric solids.

In what follows, we shall consider an isothermal approximation. We obtain the final form of the key equations by substituting the constitutive equations (16), (36), (37), geometric relations (25), and formulas (5), (14), and (15) into the balance of momentum (29), the conservation laws of induced mass (11), and Maxwell's equations (12), (13). The fundamental field equations for ideal dielectrics expressed in terms of the displacement vector $\boldsymbol{u}$, induced mass ρ_m, electric field $\boldsymbol{E}$ and magnetic induction $\boldsymbol{B}$ can be written as

$$\rho_0 \frac{\partial^2 \boldsymbol{u}}{\partial t^2} = \left(K + \frac{1}{3}G\right)\nabla(\nabla\cdot\boldsymbol{u}) + G\Delta\boldsymbol{u} - K\alpha_{E1}\nabla(\nabla\cdot\boldsymbol{E}) + 2G\alpha_{E2}\Delta\boldsymbol{E} - K\alpha_\rho\nabla\rho_m + \rho_0\boldsymbol{F}, \tag{38}$$

$$\Delta\rho_m - \frac{1}{\chi_m d_\rho}\rho_m = \frac{K\alpha_\rho}{\rho_0 d_\rho}\Delta(\nabla\cdot\boldsymbol{u}) - \frac{\beta_{E\rho}}{d_\rho}\Delta(\nabla\cdot\boldsymbol{E}) + \frac{\chi_{Em}}{\chi_m d_\rho}\nabla\cdot\boldsymbol{E}, \tag{39}$$

$$\nabla\times\boldsymbol{E} = -\frac{\partial\boldsymbol{B}}{\partial t}, \qquad \nabla\cdot\boldsymbol{B} = 0, \tag{40}$$

$$\begin{aligned}\frac{1}{\mu_0}\nabla\times\boldsymbol{B} = \sigma_e\boldsymbol{E} + \varepsilon\frac{\partial\boldsymbol{E}}{\partial t} + \rho(\chi_{q1} - \beta_{E\rho}\chi_{Em})\frac{\partial\nabla(\nabla\cdot\boldsymbol{E})}{\partial t} - 2\rho_0\chi_{q2}\frac{\partial\Delta\boldsymbol{E}}{\partial t} + \rho_0(\beta_{E\rho} - d_\rho\chi_{Em})\frac{\partial\nabla\rho_m}{\partial t}\\ + (K\alpha_\rho\chi_{Em} + \rho_0 G\alpha_{E2} - K\alpha_{E1})\frac{\partial(\nabla\nabla\cdot\boldsymbol{u})}{\partial t} + \rho_0 G\alpha_{E2}\frac{\partial\Delta\boldsymbol{u}}{\partial t},\end{aligned} \tag{41}$$

$$\begin{aligned}\varepsilon\nabla\cdot\boldsymbol{E} + \rho_0(\chi_{q1} - 2\chi_{q2} - \chi_{Em}\beta_{E\rho})\Delta(\nabla\cdot\boldsymbol{E}) + (2\rho_0 G\alpha_{E2} - K\alpha_{E1} + K\alpha_\rho\chi_{Em})\Delta(\nabla\cdot\boldsymbol{u})\\ + \rho_0(\beta_{E\rho} - d_\rho\chi_{Em})\Delta\rho_m = \rho_e.\end{aligned} \tag{42}$$

Here, $\varepsilon = \varepsilon_0 + \rho_0\chi_E$.

Note that the ponderomotive $\boldsymbol{F}_e$ and additional mass $\boldsymbol{F}_m$ forces are absent in (38) because these forces are nonlinear functions of the perturbations fields. Accounting for the local mass displacement yields an additional equation (39) in the key set and suggests modifications of (38), (41) and (42), all of which contain certain terms related to this process. Equation (39) is stationary because we consider the local mass displacement as a reversible process. Its solution depends on the sign of the coefficient $(d_\rho \chi_m)^{-1}$. From the estimation of coefficients d_ρ and χ_m it follows that these quantities are positive [Burak et al. 2011], thus, $(d_\rho \chi_m)^{-1} = \lambda_\mu^2$. Here, λ_μ^{-1} is the intrinsic length scale parameter (a material constant which dimension is length). The emergence of such a constant is typical of the gradient-type theories [Mindlin 1972], while an intrinsic length scale is absent from classical theories. As a result of accounting for the electric quadrupole, summands proportional to a second-order space partial derivative of the electric field vector $\boldsymbol{E}$ appear in the balance of momentum (38). Equations (41) and (42) change too. Now they contain summands proportional to a third-order mixed partial derivative of the electric field vector.

9. Surface energy of deformation and polarization

We apply the above relations to determine the surface energy of deformation and polarization. The notion of surface energy of deformation and polarization was originally introduced in [Mindlin 1965; 1968].

Using the constitutive equations (36), we modify expression (35) as

$$f - f_0 = \frac{1}{2\rho_0}\hat{\sigma} : \hat{\boldsymbol{e}} + \frac{1}{2}\mu'_{\pi 0}\rho_m + \frac{1}{2}\mu'_\pi \rho_m + \frac{1}{2}\boldsymbol{\pi}_m \cdot \nabla \mu'_\pi - \frac{1}{2}\boldsymbol{E}\cdot\boldsymbol{p} - \frac{1}{2}\hat{\boldsymbol{q}} : (\nabla \otimes \boldsymbol{E}). \tag{43}$$

Let us consider an equilibrium state of ideal dielectrics for which $\boldsymbol{E} = -\nabla\varphi_e$, where φ_e is electric potential. Using this formula, the equilibrium equation $\nabla\hat{\sigma} + \rho_0 \boldsymbol{F} = 0$, the geometrical relation (25), Gauss's law $(13)_2$, as well as the formulas (8) and (16), and after applying some algebra to (43), we can express the perturbation of the total energy $\mathscr{E}$ as

$$\mathscr{E} = \frac{1}{2}\rho_0\mu'_{\pi 0}\rho_m + \frac{1}{2}\rho_0 \boldsymbol{F}\cdot\boldsymbol{u} + \frac{1}{2}\nabla\cdot(\hat{\sigma}\cdot\boldsymbol{u}) - \frac{1}{2}\rho_0\nabla\cdot(\boldsymbol{\pi}_m\,\tilde{\mu}'_\pi) - \frac{1}{2}\nabla\cdot(\varphi_e \boldsymbol{D}) + \frac{1}{12}\nabla\cdot(\boldsymbol{E}\cdot\hat{\boldsymbol{Q}}). \tag{44}$$

Here, $\tilde{\mu}'_\pi = \mu'_\pi - \mu'_{\pi 0}$.

We integrate both parts of (44) over the region $(V') = (V) \cup (V_\nu)$ occupied by the body (region (V)) and vacuum (region (V_ν)). Finally, using the divergence theorem, we obtain

$$\int_{(V')} \mathscr{E}\,dV = \frac{1}{2}\rho_0\,\mu'_{\pi 0}\int_{(V)} \rho_m\,dV + \frac{1}{2}\rho_0\int_{(V)} \boldsymbol{F}\cdot\boldsymbol{u}\,dV + \frac{1}{2}\int_{(\Sigma)}\Big(\hat{\sigma}\cdot\boldsymbol{u} - \rho_0\,\boldsymbol{\pi}_m\,\tilde{\mu}'_\pi - \varphi_e[\boldsymbol{D}] + \frac{1}{6}\boldsymbol{E}\cdot\hat{\boldsymbol{Q}}\Big)\cdot\boldsymbol{n}\,d\Sigma. \tag{45}$$

Here, $[\boldsymbol{D}]$ denotes the finite jump of the electric induction over the surface (Σ).

Consider the solids with traction-free surfaces and in the absence of external forces ($\boldsymbol{F} = 0$). Then, we have $\forall \boldsymbol{r} \in (\Sigma) : \hat{\sigma}\cdot\boldsymbol{n} = 0$, and $[\boldsymbol{D}] = 0$. Hence, using formula (7), we get

$$\int_{(V)} \mathscr{E}\,dV = \frac{1}{2}\rho_0\int_{(\Sigma)} (\boldsymbol{E}\cdot\hat{\boldsymbol{q}} - \boldsymbol{\pi}_m\,\tilde{\mu}'_\pi)\cdot\boldsymbol{n}\,d\Sigma. \tag{46}$$

The righthand side of the above equality defines the surface energy of deformation and polarization U_Σ, for which in the framework of the proposed theory we obtain

$$U_\Sigma = \frac{1}{2}\rho_0(\boldsymbol{E}\cdot\hat{\boldsymbol{q}} - \boldsymbol{\pi}_m\,\tilde{\mu}'_\pi)\cdot\boldsymbol{n}\Big|_{\boldsymbol{r}\in\Sigma}. \tag{47}$$

Thus, the specific surface energy of deformation and polarization is defined by the electric field vector $\boldsymbol{E}$, the quadrupole moment $\hat{\boldsymbol{q}}$, the local mass displacement vector $\boldsymbol{\pi}_m$ and a perturbation of the modified chemical potential $\tilde{\mu}'_\pi$.

10. Surface and size effects

The linear relations of the local gradient theory of dielectrics are tested on some simple problems. In this section, they are used to study the effect of a free surface on the stress-strain state and polarization of elastic bodies having plane and cylindrical surfaces.

We apply the key set of equations (38)–(42) to investigate the near-surface inhomogeneity of electromechanical fields (i) in an infinite layer (region $|x| \le l$), (ii) in a cylinder (region $r \le R$), and (iii) in an elastic dielectric medium with a cylindrical hole (region $r \ge R$). Let as these bodies are in contact with vacuum. The body force is assumed to be zero. If we neglect the effect of electric quadrupole moments, the key set of equations can be written as

$$\left(\bar{K} + \frac{1}{3}G\right)\nabla(\nabla \cdot \boldsymbol{u}) + G\Delta\boldsymbol{u} - K\frac{\alpha_\rho}{d_\rho}\nabla\tilde{\mu}'_\pi = 0, \tag{48}$$

$$\Delta\tilde{\mu}'_\pi - \lambda_\mu^2\,\tilde{\mu}'_\pi = \lambda_\mu^2\frac{K\alpha_\rho}{\rho_0}\nabla\cdot\boldsymbol{u} + \frac{\chi_{Em}}{\chi_m}\nabla\cdot\boldsymbol{E}, \tag{49}$$

$$\nabla\cdot\boldsymbol{E} - \kappa_E\,\Delta\tilde{\mu}'_\pi = 0. \tag{50}$$

Since the body surfaces are traction-free, the boundary conditions on (Σ) ($x = \pm l$ for a layer and $r = R$ for solids of a cylindrical geometry) are

$$\hat{\sigma}\cdot\boldsymbol{n} = 0, \quad \mu'_\pi = 0, \quad \text{and } [\boldsymbol{D}] = 0. \tag{51}$$

Here $\bar{K} = K - K^2\alpha_\rho^2/(\rho_0\,d_\rho)$, and $\kappa_E = \rho_0\,\chi_{Em}/\varepsilon$.

To determine the displacement field and density of induced mass, we formulate a stationary boundary value problem, while the problem of electrodynamics is formulated as a contact problem. Therefore, the Maxwell equations in vacuum as well as the radiation conditions [Bredov et al. 1985; Nowacki 1983] should be considered together with (48)–(50).

We find analytical solutions to the problems formulated above. These solutions enable us (i) to determine the surface stresses and the surface energy of deformation and polarization in solid dielectric films and fibers, (ii) to investigate the effect of surface curvature on these values, (iii) to describe the size effects, and (iv) to justify the occurrence of a bound charge on a free surface of dielectric bodies as well as the emergence of disjoining pressure in thin solid films.

10.1. ***Layer with free boundaries.*** An analysis of the results obtained reveals that the near-surface regions of the layer are characterized by an inhomogeneous distribution of the stresses $\sigma_{yy} = \sigma_{zz} \equiv \sigma$ (Figure 2), polarization $\boldsymbol{p} = (p(x), 0, 0)$, electric field $\boldsymbol{E} = (E(x), 0, 0)$ and modified chemical $\tilde{\mu}'_\pi$

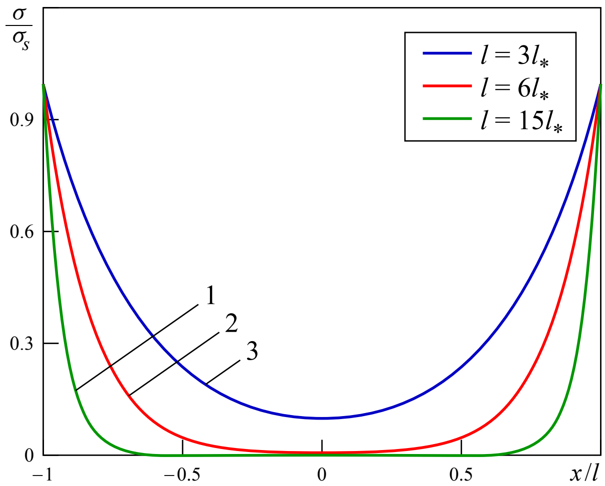

Figure 2. The distribution of the stresses σ_{yy}/σ_s in films of different thicknesses: $l = 15l_*$ (curve 1), $l = 6l_*$ (curve 2), $l = 3l_*$ (curve 3).

potentials [Burak et al. 2008]:

$$\sigma(x) = \frac{2G\rho_0\,\mathfrak{M}\,\mu'_{\pi 0}}{K\alpha_\rho}\frac{\mathrm{ch}(\breve{\lambda}x)}{\mathrm{ch}(\breve{\lambda}l)}, \qquad p(x) = \kappa_E\,\breve{\lambda}\,\mu'_{\pi 0}\frac{\varepsilon_0}{\rho_0}\frac{\mathrm{sh}(\breve{\lambda}x)}{\mathrm{ch}(\breve{\lambda}l)}, \tag{52}$$

$$\tilde{\mu}'_\pi(x) = -\mu'_{\pi 0}\frac{\mathrm{ch}(\breve{\lambda}x)}{\mathrm{ch}(\breve{\lambda}l)}, \qquad E(x) = -\kappa_E\,\breve{\lambda}\,\mu'_{\pi 0}\frac{\mathrm{sh}(\breve{\lambda}x)}{\mathrm{ch}(\breve{\lambda}l)}. \tag{53}$$

Here,

$$\breve{\lambda} = \lambda_\mu\left|\sqrt{\frac{1+\mathfrak{M}}{(1-\kappa_E\,\chi_{Em}/\chi_m)}}\right|, \qquad \mathfrak{M} = \frac{K^2\alpha_\rho^2}{\rho_0\,d_\rho(\bar{K}+4G/3)}.$$

In this case, a bound electrical charge of density $\vartheta_{se}(\pm l) = \pm\varepsilon_0\kappa_E\,\mu'_{\pi 0}\,\mathrm{th}(l/l_*)/l_*$ is induced on the surfaces of the layer $x = \pm l$ (see Figure 3, where $\vartheta_* = \varepsilon_0\kappa_E\,\mu'_{\pi 0}$, $l_* = \breve{\lambda}^{-1}$). The factors $\mathfrak{M}$ and κ_E describe the coupling between the local mass displacement and the process of deformation and the electric field, respectively [Burak et al. 2011]. Note that $\mathfrak{M}$ and κ_E are small parameters. The analysis of the results obtained also shows that layer thickness does not affect the value of surface stresses $\sigma_s = 2G\rho_0\,\mathfrak{M}\,\mu'_{\pi 0}/(K\alpha_\rho)$, but it does affect the distribution of stresses within the body [Burak et al. 2008].

The interior regions of thick layer (line 1 in Figure 2) are stress-free, while the interior regions of thin film (line 3 in Figure 2) are stressed: $\sigma(0) = \sigma_s/\,\mathrm{ch}(l/l_*)$ describes middle surface stresses. Here, we define thin films as layers with the thickness of several characteristic lengths l_*. For such films, overlaps of the regions of the near-surface inhomogeneity of fields are typical. One can see that a reduction in the film thickness leads to an increase in the stress level in the film's cross section. The dependence of the stress distribution (Figure 2) and the bound electric charge (Figure 3) on the film thickness displays their size effect.

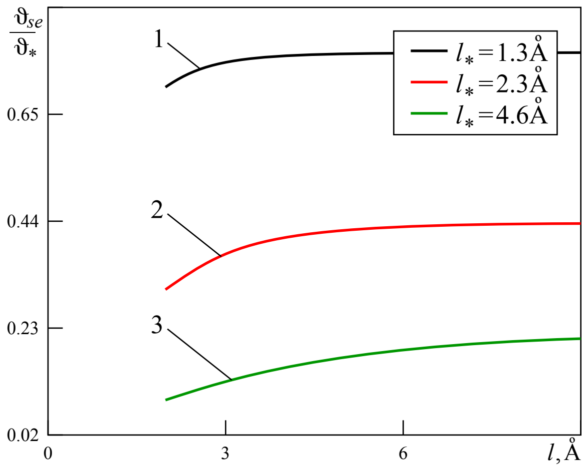

Figure 3. The dependence of the bound surface electric charge $\vartheta_{se}(l)$ on the film thickness for different materials: $l_* = 1.3$ Å (curve 1), $l = 2.3$ Å (curve 2), $l = 4.6$ Å (curve 3).

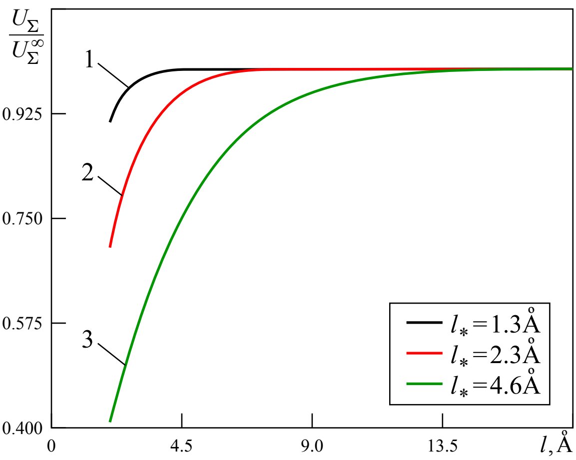

Figure 4. The dependence of the surface energy of deformation and polarization on the film thickness for different materials: $l_* = 1.3$ Å (curve 1), $l = 2.3$ Å (curve 2), $l = 4.6$ Å (curve 3).

Using (36e), (47), and (53) we obtain the formula $U_\Sigma(l) = U_\Sigma^\infty \operatorname{th}(\breve{\lambda} l)$ that describes the size effect of surface energy of deformation and polarization in thin dielectric films. Here,

$$U_\Sigma^\infty = -\rho_0\, \mu_{\pi 0}'^2 \frac{\chi_m - \kappa_E \chi_{Em}}{2 l_*},$$

is the surface energy of deformation and polarization in the half-space of the same material. The absolute value of U_Σ decreases with a decrease in the thickness of the thin film (Figure 4).

10.2. ***Solids of cylindrical geometry.*** In this subsection, the effect of surface curvature on the equilibrium stress distribution, polarization, surface energy of deformation and polarization, and bond surface electric charge is studied for dielectric bodies free from external loads. To this end, the solutions to the problems for a cylindrical fiber (region $r \le R$) and an infinite medium containing a thin cylindrical hole (region $r \ge R$) with traction-free surfaces at $r = R$ are used. The axes of the fiber and cylindrical hole coincide with the z axis. In this case the key functions $\boldsymbol{u} = (u_r(r), 0, 0)$, $\boldsymbol{E} = (E_r(r), 0, 0)$ and $\tilde{\mu}'_\pi(r)$ are functions of the space coordinate r only. Thus, the solution of boundary problem (48)–(51) is given by

$$u_r(r) = \mu'_{\pi 0} \frac{K\alpha_\rho}{\breve{\lambda} d_\rho(\bar{K} + \frac{4}{3}G)} \left[\frac{1}{2} Q\breve{\lambda} r - (1 - \mathfrak{M}Q) \frac{I_1(\breve{\lambda} r)}{I_0(\breve{\lambda} R)} \right], \tag{54}$$

$$\tilde{\mu}'_\pi(r) = -\mu'_{\pi 0} \left[(1 - \mathfrak{M}Q) \frac{I_0(\breve{\lambda} r)}{I_0(\breve{\lambda} R)} + \mathfrak{M}Q \right], \tag{55}$$

$$E_r(r) = -\kappa_E \mu'_{\pi 0} \breve{\lambda} (1 - \mathfrak{M}Q) \frac{I_1(\breve{\lambda} r)}{I_0(\breve{\lambda} R)}, \tag{56}$$

for cylindrical fiber ($r \le R$), and

$$u_r(r) = \mu'_{\pi 0} \frac{K\alpha_\rho}{\breve{\lambda}\, d_\rho(\bar{K} + \frac{4}{3}G)} \frac{K_1(\breve{\lambda} R)}{K_0(\breve{\lambda} R)} \left(\frac{K_1(\breve{\lambda} r)}{K_1(\breve{\lambda} R)} - \frac{R}{r} \right), \tag{57}$$

$$\tilde{\mu}'_\pi(r) = -\mu'_{\pi 0} \frac{K_0(\breve{\lambda} r)}{K_0(\breve{\lambda} R)}, \tag{58}$$

$$E_r(r) = \mu'_{\pi 0}\, \kappa_E\, \breve{\lambda} \frac{K_1(\breve{\lambda} r)}{K_0(\breve{\lambda} R)}, \tag{59}$$

for infinite medium with cylindrical hole ($r \ge R$). Here, I_j and K_j are the first- and second-kind modified Bessel functions of the order j (Macdonald functions), and

$$Q = -\frac{2GI_1(\breve{\lambda} R)}{(K + G/3)\breve{\lambda} R I_0(\breve{\lambda} R) - 2G\mathfrak{M} I_1(\breve{\lambda} R)}. \tag{60}$$

The analysis of the obtained solutions shows that the surface curvature has important effects on thin fibers. An increase in the surface curvature of thin fibers leads to a reduction in the density of the surface bound charge:

$$\vartheta_{se}(R) = \kappa_E\, \breve{\lambda} \varepsilon_0\, \mu'_{\pi 0} \frac{(K + G/3)\breve{\lambda} R I_1(\breve{\lambda} R)}{(K + G/3)\breve{\lambda} R I_0(\breve{\lambda} R) - 2G\mathfrak{M}\, I_1(\breve{\lambda} R)}, \tag{61}$$

as well as to an increase of the levels of absolute value of the corresponding stresses (see Figure 5, where $\mathfrak{M} = 3 \cdot 10^{-3}$, $K/G = 2.79$).

A formula that describes the influence of surface curvature on the density of the surface energy of deformation and polarization is given by

$$\frac{U^c_\Sigma}{U^\infty_\Sigma} = \begin{cases} \frac{K_1(-1/\kappa)}{K_0(-1/\kappa)}, & \kappa < 0, \\ 1, & \kappa = 0, \\ \frac{I_1(1/\kappa)}{I_0(1/\kappa) - 2G\mathfrak{M}\kappa(K+G/3)^{-1} I_1(1/\kappa)}, & \kappa > 0. \end{cases} \tag{62}$$

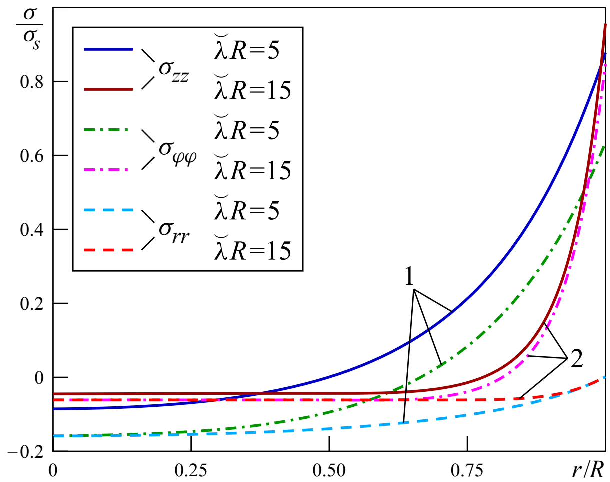

Figure 5. The effect of surface curvature on the stresses in fiber for $\breve{\lambda}R = 5$ (curve 1) and $\breve{\lambda}R = 15$ (curve 2).

Here, $\kappa = -(\breve{\lambda}R)^{-1}$ for a dielectric medium with a cylindrical hole, $\kappa = (\breve{\lambda}R)^{-1}$ for a fiber, and $\kappa = 0$ for solids with plane surfaces. An increased surface curvature of a free cylinder leads to a decrease in the absolute value of the surface energy compared to the body with a plane surface (Figure 6). By contrast, in the infinite medium with a thin cylindrical hole, an increased curvature of the surface results in an increased surface energy. Note that the characteristic lengths $l_* = 1.3$ Å and $l_* = 1.89$ Å correspond to crystals NaCl and KCl [Askar et al. 1971; Mindlin 1972]. Thus, the value of the surface energy of deformation and polarization for the body with a plane surface ($\kappa = 0$) is not the minimum of the surface energy U_Σ as a function of surface curvature.

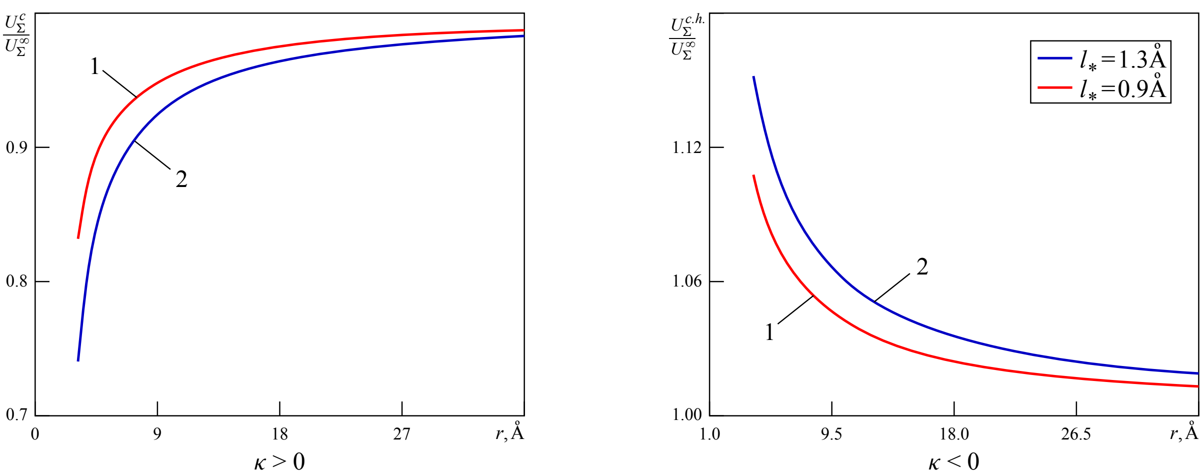

Figure 6. The effect of surface curvature on the surface energy of deformation and polarization for $l_* = 0.9$ Å (curve 1) and $l_* = 1.3$ Å (curve 2).

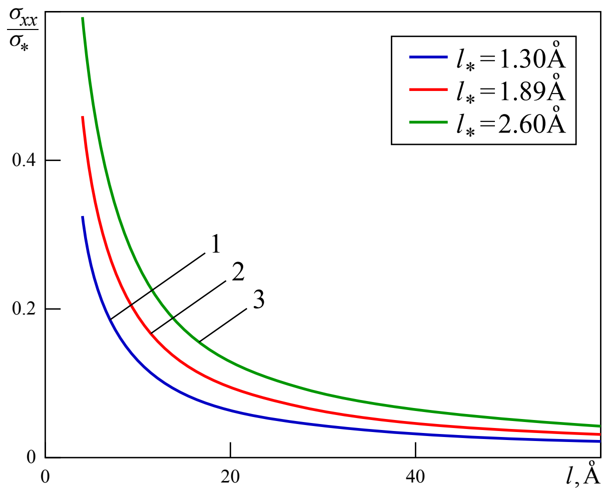

Figure 7. The dependence of the disjoining pressure on the film thickness for different materials: $l_* = 1.3$ Å (curve 1), $l_* = 1.89$ Å (curve 2), $l_* = 2.6$ Å (curve 3).

10.3. ***Layer with clamped boundaries.*** Deryagin et al. [1985] show that a disjoining pressure emerges in thin liquid films. We show that such a pressure can be present in thin solid films as well. Within the framework of the developed theory, the emergence of the disjoining pressure is associated with changes in the structure of the near-surface regions of the thin body (with the local mass displacement). To demonstrate this, within this section, we study the near-surface inhomogeneity of electromechanical fields in an infinite isotropic dielectric layer ($|x| \le l$) with clamped boundaries. Using the solutions to (48)–(50) that satisfy the boundary conditions $\boldsymbol{u} = 0$, $\mu'_\pi = 0$, and $[\boldsymbol{D}] = 0$ on the surfaces $x = \pm l$ of the layer, we investigate the stress-strain state, polarization, as well as electric and modified chemical potentials in dielectric films. In particular, for the components σ_{xx}, $\sigma_{yy} = \sigma_{zz} \equiv \sigma$ of the stress tensor we obtain

$$\sigma_{xx} = \frac{\sigma_*(1+\mathfrak{M})}{\breve{\lambda} l \,\mathrm{cth}(\breve{\lambda} l) + \mathfrak{M}}, \qquad \sigma_{yy} = \sigma_{zz} = \sigma_* \frac{\breve{\lambda} l \,\mathrm{ch}(\breve{\lambda} x) + (3K-2G)\,\mathrm{sh}(\breve{\lambda} l)/6G}{\breve{\lambda} l \,\mathrm{ch}(\breve{\lambda} l) + \mathfrak{M}\,\mathrm{sh}(\breve{\lambda} l)}. \tag{63}$$

Here, $\sigma_* = \mu'_{\pi 0} K \alpha_\rho / d_\rho$.

One can see that in films with clamped boundaries the constant normal stresses σ_{xx} appear in addition to the stresses σ_{yy} and σ_{zz}. In thick films, the stresses σ_{xx} are negligibly small, but a decreasing thickness of thin films leads to an increase of the absolute value of these stresses (Figure 7). These stresses cause a disjoining pressure in thin solid films:

$$p_{\mathrm{dis}} = \frac{1}{2l} \int_{-l}^{l} \sigma_{xx}\, dx.$$

Note also that a positive disjoining pressure can prevent the reduction of the film thickness under the effect of external forces, whereas a negative pressure can reduce the thickness of the film and thus may lead to its destruction.

11. Conclusions

It is shown that a local gradient theory of electrothermoelasticity for nonferromagnetic dielectric continua can be formulated by considering the contribution of the electric charge and mass fluxes caused by changes in material microstructure. These fluxes are (i) the nondiffusive and nonconvective mass flux, caused by a change over time of the vector of the local mass displacement (the mass dipole moment) and (ii) the electric polarization current, caused by the change over time of both the dipole and quadrupole electric moments. The result of accounting for the mentioned fluxes is an extension of the phase space of thermodynamic constitutive parameters by three additional pairs of conjugate parameters. Compared to the classical theory of dielectrics, the space of constitutive variables additionally includes: (i) the specific electric quadrupole moment $\hat{\boldsymbol{q}}$ and the gradient of the electric field vector $\nabla \otimes \boldsymbol{E}_*$; (ii) the specific density of induced mass ρ_m and the modified chemical potential μ'_π; (iii) the specific vector of the local mass displacement $\boldsymbol{\pi}_m$ and the gradient of the modified chemical potential $\nabla \mu'_\pi$. Moreover, accounting for the mentioned fluxes results in a modification of the stress tensor $\hat{\sigma}_*$ and in the emergence of a nonlinear mass force $\boldsymbol{F}_m$, in addition to the ponderomotive force $\boldsymbol{F}_e$ in the momentum equation. The effect of the force $\boldsymbol{F}_m$ can be important for investigating nonlinear effects in nanoscale films, fibers, and wires, since all of them are characterized by high gradients of physical and mechanical fields.

Within the classical linear theory of elastic dielectrics, there is no interaction between the mechanical and electromagnetic fields if the material is isotropic. Hence, flexoelectric and thermopolarization effects can occur in anisotropic materials only. Within the framework of the local gradient theory of dielectrics, the electric and thermomechanical fields are coupled. Therefore, the constitutive equations describe the polarization of the high symmetry dielectric materials (isotropic materials) caused by nonuniform deformation or by the temperature gradient (i.e., flexoelectric and thermopolarization effects).

The near-surface effects in nonferromagnetic isotropic dielectric solids are investigated to illustrate the efficiency of constructed theory. To this end, the equilibrium steady state of infinite bodies with plane-parallel and cylindrical surfaces (film, fiber, and infinite medium with a cylindrical hole) is studied within an isothermal approximation. The solutions to the formulated stationary problems allow us to describe the experimental data reported in the literature, namely, the near-surface inhomogeneity of electromechanical fields, the emergence of a bound electric charge on the free surfaces of the dielectric bodies, as well as the size effects of the stresses, bound electric charge, surface energy of deformation and polarization. It is established that the absolute value of the surface charge density decreases and mechanical stresses increases when thin film thickness decreases. This effect became more significant when the film thickness became comparable to the internal material length scale parameters.

As the curvature of the surface increases, its impact on the stressed state of thin fibers and on the value of the bound charge on their surfaces becomes more significant. An increase in the surface curvature of thin cylindrical fiber leads to increased levels of stresses and to a reduced density of the surface bound charge. The influence of the curvature on the surface energy of deformation and polarization depends on the curvature sign. Namely, an increase in the absolute value of a positive curvature leads to a decrease in the absolute value of this energy. For a negative curvature, this dependence is reversed.

The theory also implies the emergence of disjoining pressure in thin solid films. The existence of such pressure was previously anticipated in liquid films [Deryagin et al. 1985]. It is shown that in thin solid films, whose thickness is comparable to the internal material length scale parameters, the disjoining pressure can appear. This pressure is proportional to the coefficient of volume dilatation caused by the local mass displacement. The absolute value of disjoining pressure increases if the mentioned coefficient increases. In light of this finding, during an investigation of the stiffness and strength of nanoscale thin films, the effect of the disjoining pressure on the abovementioned parameters should be considered.

The results obtained in the paper are general and can be useful for the design of the devices utilizing the micro/nanofilm elements.

List of symbols

ρ	mass density
$\rho_{m\pi}$	density of induced mass
ρ_m	specific density of induced mass
$\rho_{e\pi}$	density of induced charge
ρ_e	density of free charges
T	absolute temperature
t	time variable
s	specific entropy
$\mathfrak{R}$	distributed heat source
η	entropy production
$\mathscr{E}$	total energy
u	specific internal energy
U_e	electromagnetic field energy
U_Σ	surface energy of deformation and polarization
f	Helmholtz free energy
μ	chemical potential
μ_π	energy measure of the effect of the local mass displacement on the internal energy
φ_e	electric potential
ϑ_{se}	density of bound electrical charge
$\boldsymbol{J}_q$	density of heat flux
$\boldsymbol{J}_{ef}$	density of total electric current
$\boldsymbol{J}_e$	density of electric current (convection and conduction currents)
$\boldsymbol{J}_{es}$	polarization current
$\boldsymbol{J}_{m^*}$	density of mass flux
$\boldsymbol{J}_{ms}$	nonconvective and nondiffusive mass flux related to local mass displacement
$\boldsymbol{S}_e$	flux of electromagnetic energy
$\boldsymbol{\Pi}_m$	vector of local mass displacement (mass dipole moment)
$\boldsymbol{\Pi}_e$	polarization vector
$\boldsymbol{P}$, $\hat{\boldsymbol{Q}}$	dipole and quadrupole electric moments
$\boldsymbol{E}$, $\boldsymbol{H}$	electric and magnetic fields
$\boldsymbol{D}$, $\boldsymbol{B}$	electric and magnetic inductions
$\boldsymbol{v}_*$	velocity vector of convective displacement of the fixed body element
$\boldsymbol{v}$	velocity vector of the center of mass
$\boldsymbol{r}$	position vector
$\boldsymbol{F}$	mass forces
$\boldsymbol{F}_e$	ponderomotive force
$\hat{\sigma}$	Cauchy stress tensor
$\hat{\boldsymbol{e}}$	infinitesimal strain tensor

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