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THE CONSTITUTIVE EQUATIONS OF LOCAL GRADIENT THEORY OF ANISOTROPIC DIELECTRICS

Yaroslav BURAK, Olha HRYTSYNA
Institute of Applied Problems of Mechanics and Mathematic of NAS of Ukraine,
Center of Mathematical Modelling of Institute of Applied Problems of Mechanics and Mathematic of NAS of Ukraine, Lviv

1. Introduction

One of the important areas of modern continuum mechanics is the study of problems related to surface and size effects. To describe these effects in dielectrics non-local theories [1, 2] have been effectively used for more than half a century. These theories assume that the state of a fixed point of body depends on the state of the neighbouring points. Non-local theories of dielectrics assume the constitutive relations of integral type [3] or take into account the dependence of the body state on strain gradients [4], polarization gradient [5], electric field gradients or higher electric moments (quadrupoles, octupoles and so on) [6, 7]. Another approach to the formation of non-local theory of dielectrics was proposed in papers [8, 9]. This approach is based on accounting the process of local mass displacement [10] apart from deformation process, thermal conductivity and polarization. The process of local mass displacement was associated with the possible structural changes within the fixed body element. Structural displacement of the mass center of fixed body elements occurs in the vicinity of newly created surfaces. The account of the process of local mass displacement leads to constitutive equations typical of gradient-type theories. A complete set of equations of local gradient theory of nonferromagnetic dielectrics for isotropic materials was obtained in [8]. In the present paper, we extend the local gradient theory of electro-magneto-thermo-mechanics to dielectric materials of an arbitrary symmetry.

2. The basic relations of local gradient theory of dielectrics

We consider a thermo-elastic polarized nonferromagnetic solid, which is subjected to the action of an external load, which induces mechanical, thermal and electromagnetic processes and causes the ordering of body structure and electric charge. The Maxwell's equations may be represented as [11, 12]

$$\nabla\cdot\mathbf{B}=0\,,\qquad \nabla\cdot\mathbf{D}=\rho_e\,,\qquad \nabla\times\mathbf{E}=-\frac{\partial\mathbf{B}}{\partial t}\,,\qquad \nabla\times\mathbf{H}=\mathbf{J}_e+\varepsilon_0\frac{\partial\mathbf{E}}{\partial t}+\mathbf{J}_{es}\,. \qquad (1)$$

Here $\mathbf{J}_{es} = \dfrac{\partial \mathbf{P}}{\partial t}$ is the polarization current. Together with the polarizing currents $\mathbf{J}_{es}$, caused by ordering of charge system, we will also take into account the non-convective and non-diffusive mass fluxes $\mathbf{J}_{ms}$ of similar nature. Therefore, in the equation of mass balance we regard that a displacement of the mass center of fixed body element can be caused by convection of this element and by structural changes that are not associated with diffusive processes. The process, which takes into account such mass fluxes, was referred to as a process of local mass displacement. Taking into account this process, the equation of mass conservation can be expressed as [8] $\dfrac{\partial \rho}{\partial t} = -\nabla \cdot \left(\rho \mathbf{v}_* + \mathbf{J}_{ms} \right)$, where $\mathbf{v}_*$ is velocity of convective displacement of the fixed body element. We introduce the vector of local mass displacement by formula: $\mathbf{\Pi}_m \left(\mathbf{r}, t \right) = \int_0^t \mathbf{J}_{ms} \left(\mathbf{r}, t' \right) dt'$. For vector $\mathbf{J}_{ms}$ one obtains: $\mathbf{J}_{ms} = \partial \mathbf{\Pi}_m / \partial t$. The velocity vector $\mathbf{v}$ of the centre of mass is defined by relation: $\mathbf{v} = \rho^{-1} \left(\rho \mathbf{v}_* + \partial \mathbf{\Pi}_m / \partial t \right)$. Then, the equation of mass balance acquires a standard form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 . \tag{2}$$

In order to describe the local mass displacement, we have introduced the potential μ_π being the energy measure of the effect of aforementioned process on the internal energy. Similarly to the induced electric charge [11], we have introduced the density of induced mass $\rho_{m\pi}$ [8, 9]. It is required that for an arbitrary solid of finite size (domain (V)), the vector of local mass displacement $\mathbf{\Pi}_m$ and density of the induced mass $\rho_{m\pi}$ should satisfy the following integral relation: $\int_{(V)} \mathbf{\Pi}_m dV = \int_{(V)} \rho_{m\pi} \mathbf{r} dV$ [8]. From this relation we deduce that $\rho_{m\pi} = -\nabla \cdot \mathbf{\Pi}_m$. It is easy to show that equation

$$\frac{\partial \rho_{m\pi}}{\partial t} + \nabla \cdot \mathbf{J}_{ms} = 0 \tag{3}$$

is satisfied. This equation has the form of the conservation law of induced mass.

The momentum equation [8] and entropy balance equation [13] are as follows:

$$\rho \frac{d\mathbf{v}}{dt} = \nabla \cdot \hat{\boldsymbol{\sigma}}_* + \mathbf{F}_e + \rho \mathbf{F}_* , \qquad \rho T \frac{ds}{dt} = -\nabla \cdot \mathbf{J}_q + \frac{1}{T} \mathbf{J}_q \cdot \nabla T + T \sigma_s + \rho \Re . \tag{4}$$

Here $\mathbf{F}_e = \rho_e \mathbf{E}_* + \left(\mathbf{J}_{e*} + \dfrac{\partial (\rho \mathbf{p})}{\partial t} \right) \times \mathbf{B} + \rho \left(\nabla \mathbf{E}_* \right) \cdot \mathbf{p}$, $\mathbf{F}_* = \mathbf{F} + \rho_m \nabla \mu'_\pi - \boldsymbol{\pi}_m \cdot \nabla \nabla \mu'_\pi$, $\hat{\boldsymbol{\sigma}}_* = \hat{\boldsymbol{\sigma}} - -\rho \left(\mathbf{E}_* \cdot \mathbf{p} - \rho_m \mu'_\pi - \boldsymbol{\pi}_m \cdot \nabla \mu'_\pi \right) \hat{\mathbf{I}}$, $\mathbf{E}_* = \mathbf{E} + \mathbf{v} \times \mathbf{B}$, $\mathbf{J}_{e*} = \mathbf{J}_e - \rho_e \mathbf{v}$, $\mu'_\pi = \mu_\pi - \mu$, $\mathbf{p} = \mathbf{P} / \rho$, $\boldsymbol{\pi}_m = \mathbf{\Pi}_m / \rho$, $\rho_m = \rho_{m\pi} / \rho$ and $d\ldots / dt = \partial \ldots / \partial t + \mathbf{v} \cdot \nabla \ldots$. In previous papers [8, 9] we have obtained the following relation for entropy production: $\sigma_s = \mathbf{J}_{e*} \cdot \dfrac{\mathbf{E}_*}{T} - \mathbf{J}_q \cdot \dfrac{\nabla T}{T^2}$.

A complete set of equations of local gradient theory of dielectrics together with Maxwell equations (1) and balance equations (2)-(4) should include corresponding physical and geometric relations. In the present paper, we obtain the physical relationships of local gradient theory of anisotropic nonferromagnetic dielectrics.

3. The constitutive equations for an anisotropic medium

Having taken into account the process of local mass displacement we have obtained the generalized Gibbs equation $df = \rho^{-1}\hat{\boldsymbol{\sigma}}_* : d\hat{\boldsymbol{e}} - s dT - \mathbf{p}\cdot d\mathbf{E}_* + \mu'_\pi d\rho_m + \boldsymbol{\pi}_m \cdot d\left(\nabla\mu'_\pi\right)$ [8], which contains two pairs of additional state parameters, namely: (i) the specific density of induced mass ρ_m and the potential μ'_π, and (ii) the specific vector of local mass displacement $\boldsymbol{\pi}_m$ and vector $\nabla\mu'_\pi$. From the Gibbs relation we get the following constitutive equations

$$\hat{\boldsymbol{\sigma}}_* = \rho\frac{\partial f}{\partial \hat{\mathbf{e}}}, \quad s = -\frac{\partial f}{\partial T}, \quad \mu'_\pi = \frac{\partial f}{\partial \rho_m}, \quad \mathbf{p} = -\frac{\partial f}{\partial \mathbf{E}_*}, \quad \boldsymbol{\pi}_m = \frac{\partial f}{\partial\left(\nabla\mu'_\pi\right)}. \tag{5}$$

Let us decompose the free energy f into a series in perturbations of state parameters with respect to the original state of homogenous anisotropic medium with $\hat{\boldsymbol{e}} = 0$, $\hat{\boldsymbol{\sigma}}_* = 0$, $T = T_0$, $s = s_0$, $\mathbf{E}_* = 0$, $\mathbf{p} = 0$, $\nabla\mu'_\pi = 0$, $\boldsymbol{\pi}_m = 0$, $\rho_m = 0$ and $\mu'_\pi = \mu'_{\pi 0}$. For small perturbations, we retain quadratic terms in this decomposition. Within this approximation $\mathbf{E}_* = \mathbf{E}$. Hence ,

$$\begin{aligned} f = {} & f_0 - s_0\theta + \mu'_{\pi 0}\rho_m + \frac{1}{2\rho_0}\left(\hat{\mathbf{C}}^{(4)} : \hat{\boldsymbol{e}}\right) : \hat{\boldsymbol{e}} - \frac{C_V}{2T_0}\theta^2 + \frac{1}{2}d_\rho\rho_m^2 - \frac{1}{\rho_0}\left(\hat{\boldsymbol{\beta}} : \hat{\boldsymbol{e}}\right)\theta - \frac{1}{\rho_0}\left(\hat{\boldsymbol{\alpha}}^\rho : \hat{\boldsymbol{e}}\right)\rho_m - \\ & -\beta_{T\rho}\rho_m\theta - \frac{1}{\rho_0}\left(\hat{\mathbf{f}}^{(3)} : \hat{\boldsymbol{e}}\right)\cdot\mathbf{E} - \frac{1}{\rho_0}\left(\hat{\mathbf{g}}^{(3)} : \hat{\boldsymbol{e}}\right)\cdot\nabla\mu'_\pi - \left(\boldsymbol{\beta}^E\cdot\mathbf{E}\right)\theta - \left(\boldsymbol{\beta}^\mu\cdot\nabla\mu'_\pi\right)\theta - \frac{1}{2}\left(\hat{\boldsymbol{\chi}}^E\cdot\mathbf{E}\right)\cdot\mathbf{E} - \\ & - \frac{1}{2}\left[\hat{\boldsymbol{\chi}}^m\cdot\left(\nabla\mu'_\pi\right)\right]\cdot\left(\nabla\mu'_\pi\right) + \left(\hat{\boldsymbol{\chi}}^{Em}\cdot\mathbf{E}\right)\cdot\left(\nabla\mu'_\pi\right) - \left(\boldsymbol{\gamma}^E\cdot\mathbf{E}\right)\rho_m - \left(\boldsymbol{\gamma}^\rho\cdot\nabla\mu'_\pi\right)\rho_m . \end{aligned} \tag{6}$$

Here $\theta = T - T_0$ is the temperature change with respect to the reference temperature. Note that indexes in brackets denote the rank of third and fourth valency tensors (at tensors of first, second and third valence, these indexes are absent). Using the formulas (5), (6) the constitutive equations for anisotropic materials can be written as follows:

$$\hat{\boldsymbol{\sigma}}_* = \hat{\mathbf{C}}^{(4)} : \hat{\boldsymbol{e}} - \hat{\boldsymbol{\beta}}\theta - \hat{\boldsymbol{\alpha}}^\rho\rho_m - \mathbf{E}\cdot\hat{\mathbf{f}}^{(3)} - \nabla\mu'_\pi\cdot\hat{\mathbf{g}}^{(3)}, \tag{7}$$

$$s = s_0 + C_V T_0^{-1}\theta + \beta_{T\rho}\rho_m + \boldsymbol{\beta}^\mu\cdot\nabla\mu'_\pi + \boldsymbol{\beta}^E\cdot\mathbf{E} + \rho_0^{-1}\hat{\boldsymbol{\beta}} : \hat{\boldsymbol{e}}, \tag{8}$$

$$\mu'_\pi = \mu'_{\pi 0} + d_\rho\rho_m - \beta_{T\rho}\theta - \boldsymbol{\gamma}^E\cdot\mathbf{E} - \boldsymbol{\gamma}^\rho\cdot\nabla\mu'_\pi - \rho_0^{-1}\hat{\boldsymbol{\alpha}}^\rho : \hat{\boldsymbol{e}}, \tag{9}$$

$$\mathbf{p} = \hat{\boldsymbol{\chi}}^E\cdot\mathbf{E} - \hat{\boldsymbol{\chi}}^{Em}\cdot\left(\nabla\mu'_\pi\right) + \boldsymbol{\beta}^E\theta + \boldsymbol{\gamma}^E\rho_m - \rho_0^{-1}\hat{\mathbf{f}}^{(3)} : \hat{\boldsymbol{e}}, \tag{10}$$

$$\boldsymbol{\pi}_m = -\hat{\boldsymbol{\chi}}^m\cdot\left(\nabla\mu'_\pi\right) + \hat{\boldsymbol{\chi}}^{Em}\cdot\mathbf{E} - \boldsymbol{\gamma}^\rho\rho_m - \boldsymbol{\beta}^\mu\theta - \rho_0^{-1}\hat{\mathbf{g}}^{(3)} : \hat{\boldsymbol{e}}, \tag{11}$$

where $\hat{\mathbf{C}}^{(4)}$ is the fourth-rank tensor of elastic moduli; $\hat{\boldsymbol{\beta}}$ is the tensor of thermal expansion coefficients; $\hat{\boldsymbol{\alpha}}^{\rho}$ is tensor of volumetric expansion caused by local mass displacement; $\hat{\mathbf{f}}^{(3)}$ and $\hat{\mathbf{g}}^{(3)}$ are the third-rank tensors of piezoelectric and piezomass coefficients; C_V is the specific heat at constant volume; $\beta_{T\rho}$ is the coefficient of dependence of entropy on specific density of reduced mass; $\boldsymbol{\beta}^E$ and $\boldsymbol{\beta}^{\mu}$ are the pyroelectric and pyromass coefficients; d_{ρ} the coefficient of dependence of potential μ'_{π} on specific density of reduced mass; $\hat{\boldsymbol{\chi}}^E$ the tensor of dielectric susceptibility; $\hat{\boldsymbol{\chi}}^m$ and $\hat{\boldsymbol{\chi}}^{Em}$ are the tensors characterizing the dependence of vectors of local mass displacement and polarization on $\nabla\mu'_{\pi}$; $\boldsymbol{\gamma}^{\rho}$ and $\boldsymbol{\gamma}^E$ are the coefficiens characterizing the dependence of potentias μ'_{π} on its gradient ($\nabla\mu'_{\pi}$) and on the vector of electric field. It is noted that $\mu'_{\pi 0}$, d_{ρ}, $\beta_{T\rho}$, $\boldsymbol{\beta}^{\mu}$, $\boldsymbol{\gamma}^E$, $\boldsymbol{\gamma}^{\rho}$, $\hat{\boldsymbol{\alpha}}^{\rho}$, $\hat{\boldsymbol{\chi}}^m$, $\hat{\boldsymbol{\chi}}^{Em}$ and $\hat{\mathbf{g}}^{(3)}$ are new coefficients appearing in local gradient theory of thermoelasticity of nonferromagnetic dielectrics.

The fourth-rank tensor of elastic moduli $\hat{\mathbf{C}}^{(4)}$ contains, in general, 81 coeficients, each third-rank tensor of piezoelectric $\hat{\mathbf{f}}^{(3)}$ and piezomass $\hat{\mathbf{g}}^{(3)}$ coefficients contains 27 components, each tensor of second valence $\hat{\boldsymbol{\alpha}}^{\rho}$, $\hat{\boldsymbol{\beta}}$, $\hat{\boldsymbol{\chi}}^E$, $\hat{\boldsymbol{\chi}}^m$, and $\hat{\boldsymbol{\chi}}^{Em}$ has 9 components and each vector $\boldsymbol{\beta}^{\mu}$, $\boldsymbol{\beta}^E$, $\boldsymbol{\gamma}^E$, $\boldsymbol{\gamma}^{\rho}$ has 3 components. It is easy to show that the number of tensor components $\hat{\mathbf{C}}^{(4)}$, $\hat{\mathbf{f}}^{(3)}$, $\hat{\mathbf{g}}^{(3)}$, $\hat{\boldsymbol{\alpha}}^{\rho}$ and $\hat{\boldsymbol{\beta}}$ decreases if we take into account the symmetry of the stress and strain tensors. Indeed, from condition of tensor symmetry, we obtain the equalities: $C_{ijkl} = C_{jikl}$, $C_{ijkl} = C_{jilk}$, $f_{kij} = f_{kji}$, $g_{kij} = g_{kji}$, $\beta_{ij} = \beta_{ji}$ and $\alpha^{\rho}_{ij} = \alpha^{\rho}_{ji}$. Moreover, since the Gibbs equation is written for the total differential of function f, the following conditions should be satisfied

$$\frac{\partial^2 f}{\partial e_{ij}\partial e_{kl}} = \frac{\partial^2 f}{\partial e_{kl}\partial e_{ij}}, \quad \frac{\partial^2 f}{\partial E_i \partial E_j} = \frac{\partial^2 f}{\partial E_j \partial E_i},$$
$$\frac{\partial^2 f}{\partial(\nabla_i\mu'_{\pi})\partial(\nabla_j\mu'_{\pi})} = \frac{\partial^2 f}{\partial(\nabla_j\mu'_{\pi})\partial(\nabla_i\mu'_{\pi})}, \quad \frac{\partial^2 f}{\partial E_i \partial(\nabla_j\mu'_{\pi})} = \frac{\partial^2 f}{\partial(\nabla_j\mu'_{\pi})\partial E_i}. \tag{13}$$

Using the formulas (5) and (13) we get

$$\frac{\partial\sigma_{*ij}}{\partial e_{kl}} = \frac{\partial\sigma_{*kl}}{\partial e_{ij}}, \quad \frac{\partial p_i}{\partial E_j} = \frac{\partial p_j}{\partial E_i}, \quad \frac{\partial\pi_{mi}}{\partial(\nabla_j\mu'_{\pi})} = \frac{\partial\pi_{mj}}{\partial(\nabla_i\mu'_{\pi})}, \quad -\frac{\partial p_i}{\partial(\nabla_j\mu'_{\pi})} = \frac{\partial\pi_{mj}}{\partial E_i}.$$

From these formulas it follows that $C_{ijkl} = C_{klij}$, $\chi^E_{ij} = \chi^E_{ji}$, $\chi^m_{ij} = \chi^m_{ji}$ and $\chi^{Em}_{ij} = \chi^{Em}_{ji}$. Thus, the number of independent components of elastic moduli tensor $\hat{\mathbf{C}}^{(4)}$ decreased to 21. Each third-rank tensor, $\hat{\mathbf{f}}^{(3)}$ and $\hat{\mathbf{g}}^{(3)}$, has 18 independent components (they are symmetrical relatively to permutation of second and third indexes) and each tensor $\hat{\boldsymbol{\alpha}}^{\rho}$, $\hat{\boldsymbol{\beta}}$, $\hat{\boldsymbol{\chi}}^E$, $\hat{\boldsymbol{\chi}}^m$ and

$\hat{\boldsymbol{\chi}}^{Em}$ has 6 independent components. Note that all components of third-rank tensors $\hat{\mathbf{f}}^{(3)}$ and $\hat{\mathbf{g}}^{(3)}$ are equal to zero for isotropic materials. Components of the second valence tensors become: $\alpha_{ij} = \gamma_p \delta_{ij}$, $\beta_{ij} = \gamma_T \delta_{ij}$, $\chi_{ij}^E = \chi_E \delta_{ij}$, $\chi_{ij}^m = \chi_m \delta_{ij}$, $\chi_{ij}^{Em} = \chi_{Em}\delta_{ij}$ while for elastic moduli tensor $\mathbf{C}^{(4)}$ we have: $C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu\left(\delta_{jk}\delta_{il} + \delta_{ik}\delta_{jl}\right)$, $\lambda \equiv C_{1122}$ and $\mu \equiv \left(C_{1111} - C_{1122}\right)/2$, where λ and μ are the Lamé moduli.

Along with the thermodynamic parameters of state we also introduce thermodynamic parameters of processes, namely, the thermodynamic fluxes $\mathbf{j}_k$ and thermodynamic forces $\mathbf{X}_k$ that characterize the intensity of thermodynamic processes and the cause of emerging thereof. To determine these values, we rewrite the equation for entropy production as follows: $\sigma_s = \sum_{k=1}^{2} \mathbf{j}_k \cdot \mathbf{X}_k$. Here $\mathbf{j}_1 = \mathbf{J}_q$, $\mathbf{X}_1 = -T^{-2}\nabla T$, $\mathbf{j}_2 = \mathbf{J}_{e*}$ and $\mathbf{X}_2 = T^{-1}\mathbf{E}_*$. Since thermodynamic forces cause thermodynamic fluxes, we define the fluxes as functions of thermodynamic forces [13]: $\mathbf{j}_i = \mathbf{j}_i\left(\mathbf{X}_1, \mathbf{X}_2\right)$, $i = 1, 2$. Assuming this relation to be linear we obtain the following kinetic equations

$$\mathbf{J}_q = -\frac{1}{T^2}\hat{\mathbf{L}}_T \cdot \nabla T + \frac{1}{T}\hat{\mathbf{L}}_{TE} \cdot \mathbf{E}, \quad \mathbf{J}_{e*} = -\frac{1}{T^2}\hat{\mathbf{L}}_{ET} \cdot \nabla T + \frac{1}{T}\hat{\mathbf{L}}_E \cdot \mathbf{E}. \qquad (13)$$

Here $\hat{\mathbf{L}}_T$, $\hat{\mathbf{L}}_E$, $\hat{\mathbf{L}}_{TE}$ and $\hat{\mathbf{L}}_{ET}$ are the kinetic coefficients (the second-rank order tensors).

Let us consider a state of anisotropic nonferromagnetic dielectrics in the absence of mechanical, heat and electromagnetic loads. In this case there are no deformations, perturbations of temperature and electric field in dielectrics. From relations (7), (8) and (10) it follows that such a system even in the absence of external action will be polarized $\left(\mathbf{p}' = \boldsymbol{\gamma}^E \rho_m - \hat{\boldsymbol{\chi}}^{Em} \cdot \left(\nabla\mu'_\pi\right)\right)$. In this system there are stresses $\left(\hat{\boldsymbol{\sigma}}'_* = -\nabla\mu'_\pi \cdot \hat{\mathbf{g}}^{(3)} - \hat{\boldsymbol{\alpha}}^\rho \rho_m\right)$ and entropy perturbation $\left(s' - s_0 = \beta_{T\rho}\rho_m + \boldsymbol{\beta}^\mu \cdot \nabla\mu'_\pi\right)$, which is caused by structure changes of a fixed body element.

Nomenclature

$\hat{\boldsymbol{\sigma}}$ is Cauchy's stress tensor,
$\hat{\boldsymbol{e}}$ is strain tensor,
$\mathbf{F}$, $\mathbf{r}$ are mass force and position vectors,
$\mathbf{E}$, $\mathbf{H}$ are electric and magnetic fields,
$\mathbf{B}$, $\mathbf{D}$ are vectors of electric and magnetic inductions,
$\mathbf{P}$ is local displacement of electric charge (polarization),
ρ_e is density of free electric charge
ε_0, μ_0 are electric and magnetic constants,
$\mathbf{J}_e$ is density of electric current,
t is time,
T, s are absolute temperature and specific entropy,

σ_s , $\Re$ are entropy production and distributed thermal sources,

$\mathbf{J}_q$ is density of heat flux,

ρ , μ are mass density and chemical potential,

T_0 , s_0 are temperature and entropy in reference state,

ρ_0 , $\mu'_{\pi 0}$ are mass density and reduced potential μ'_π in reference state,

$\hat{\mathbf{I}}$, ∇ are unit tensor and Hamilton operator.

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RÓWNANIA KONSTYTUTYWNE LOKALNIE GRADIENTOWEJ TEORII ANIZOTROPOWYCH DIELEKTRYKÓW

Streszczenie

W oparciu o metody termodynamiki procesów nieodwracalnych otrzymano równania konstytutywny lokalnie gradientowej teorii nieferromagnetic anizotropowych dielektrykow. Ustalono, że proponowana teoria daje możliwość do opisania niejednorodności naprężeń, odkształceń i elektrycznej polaryzacji w otoczeniu powierzchni anizotropowych dielektrycznych ciał.