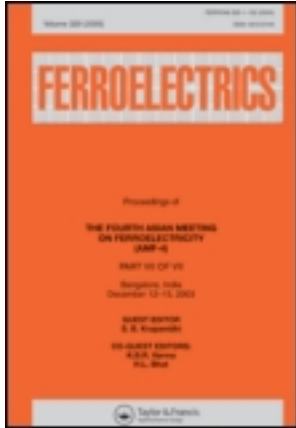


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Account for Mutual Influence of Electrical, Elastic, and Thermal Phenomena for Ferroelectric Domain Wall Modeling

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The theoretical model of the ferroelectric domain wall motion has been developed. It is demonstrated that for a proper phenomenon description it is necessary to consider the thermoelectroelasticity gradient terms. It is shown that in the linear approximation the general solution of three-dimensional problem in transversely isotropic thermoelectroelastic media can be obtained by means of five newly introduced harmonic potential functions. As an example of the proposed model applicability, the electroelastic field induced by a sphere (SPM tip) located near a plane boundary of two half-spaces is considered and described.

Keywords Ferroelectric; domain wall; domain switching; SPM; approximate boundary conditions

I. Introduction

It is a well-established fact that for the description of the ferroelectric behavior it is necessary to consider the electric and elastic fields simultaneously [1–5]. At the same time, the influence of thermal phenomena has not been discussed in the literature before. In this work we have shown that the account of latter ones is essential in the context of proper modeling of ferroelectric materials. A complete theory of the domain wall should take into account the interaction of electromagnetic, elastic, and thermal fields. Moreover, the influence of the magnetic field, caused by the presence of currents having different nature, should be taken into account even in the case of non-multiferroics ferroelectric. To be more precise, there are the typical “electric” current induced by the polarization change, pyroelectric current, which appears for the varying temperature [6], and, finally, piezoelectric current caused by the change of elastic stresses. We restrict ourselves by description of the electrical, thermal, and elastic fields interaction only. Taking into account the magnetic field contribution, the developed approach can easily be accomplished by introducing of additional terms. However, such a procedure leads to a significant complication of the formulas. For example, the number of the possible gradient terms increases from 6 to 12. We admit the necessity

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to take these terms into consideration, but this is out of the scope of this work. In the case of the domain wall motion the change of the polarization takes place in a small area. This fact, due to the electrocaloric effect, results in the release or absorption of heat at the domain interface. It is possible to estimate temperature change caused by the electrocaloric effect in 0.1 K [7] and the size of the heating area of 10 nm [3]. From analysis of this data one may conclude that a temperature gradient is of 10^7 K/m that coincides with the order of magnitude of the temperature gradients in the burning film. Moreover, it is obvious that the consideration of the elastic field gradient at the domain wall is also necessary. As a consequence, flexoelectric and flexothermal effects must be simultaneously taken into account.

II. Statement of the Problem

For simultaneous description of electrical, thermal, and elastic properties of ferroelectric we introduce the following physical quantities: the potential ϕ , the vector of polarization \vec{P} , the electric field $\vec{E} = -\nabla\phi$, the dielectric displacement $\vec{D} = \varepsilon_0\vec{E} + \vec{P}$, the vector of deformation u_i ($i = 1,2,3$), the strain tensor $\varepsilon_{ij} = (u_{i,k} + u_{k,i})/2$, and the stress tensor σ_{ij} . Here and below, the symbol $\chi_{i,k}$ means $\partial\chi_i/\partial x_k$. Further, we will use Einstein's notation for the summation of repeated indices.

The generalized form of the free energy density is given by:

$$F = F_0(T) + F_{\text{Landau}} + F_{\text{elast}} + F_{\text{grad}} + F_{\text{coup}} + F_{\text{coupgrad}}, \quad (1)$$

where $F_0(T)$ is the independent on field part of the free energy. The second and third summands in Eq. (1) are Landau potential and the elastic part of the free energy containing the thermal stress tensor, respectively. The Landau thermodynamic potential can be written in the form [3]:

$$F_{\text{Landau}} = \frac{a_i}{2} P_i^2 + \frac{a_{ij}}{4} P_i^2 P_j^2 + \frac{a_{ijk}}{6} P_i^2 P_j^2 P_k^2 - E_i P_i, \quad (2)$$

which allows to describe phase transitions of the first and the second kind. Among the Ginzburg-Landau coefficients $\{a_i, a_{ij}, a_{ijk}\}$, only the first one depends on the temperature: $a_i = a_{i0}(T - T_c)$, where a_{i0} is the Curie-Weiss constant. The elastic part of the free energy is:

$$F_{\text{elast}} = c_{ijkl}\varepsilon_{ij}\varepsilon_{kl} + (T - T_0)t_{ij}\varepsilon_{ij}, \quad (3)$$

where c_{ijkl} is the elastic modules tensor and t_{ij} is the thermal stress tensor, while T_0 is ambient temperature. The gradient terms can be represented as:

$$F_{\text{grad}} = \lambda_{ij}T_iT_j + g_{ijkl}D_{i,j}D_{k,l}, \quad (4)$$

where λ_{ij} is the thermal conductivity tensor, while g_{ijkl} are electrical gradient tensor coefficients. Let us mention that Eq. (4) includes the components of the electric displacement \vec{D} instead of the polarization \vec{P} (as performed in the standard approach [3]). This is because the presence of $(\nabla\vec{P})^2$ in Eq. (4) results in the continuity of \vec{P} normal component at the interface, contradicting Maxwell's equations. Piezoelectric part of the free energy can be expressed by the formula [9]:

$$F_{\text{coup}} = e_{ijk}\varepsilon_{ij}P_k + e_{ijkl}\varepsilon_{ij}P_kP_l, \quad (5)$$

where e_{ijk} is the piezoelectric constants tensor and e_{ijkl} are modules of the electrostriction. The first term in Eq. (5) describes the piezoelectric effect, which exists under certain restrictions on the symmetry of the ferroelectric material. The second term is responsible for the electrostriction. In the last summand of the free energy we collect the terms, which describe the influence on the polarization and temperature (as well as strain gradients of these quantities):

$$F_{\text{coupgrad}} = b_{ij} P_i T_{,j} + b_{ijk} \varepsilon_{ij} T_{,k} + f_{ijk} (T - T_0) \varepsilon_{ijk} + f_{ijkl} P_i \varepsilon_{jk,l} + d_{ijkl} \varepsilon_{ij} P_{k,l} + d_{ij} (T - T_0) P_{i,j}. \quad (6)$$

There exist six possible variants of the pair-wise interaction for three variables $\{\vec{P}, T, \varepsilon_{ij}\}$ and their gradients (any interactions between the quantity and its gradient are not considered). In other words, the first couple of terms in Eq. (6) describe the impact of ∇T on the polarization (the thermopolarization effect or polarization thermogradient effect) and the strain (the elastic thermogradient effect). The second pair reflects the impact of the strain gradient on the temperature (the flexothermal effect) and polarization (the flexoelectric effect). The third pair is used to describe the polarization dependence on the temperature gradient and deformation (thermal and elastic polarization gradient effects). The quantities $\{b_{ij}, b_{ijk}, f_{ijk}, f_{ijkl}, d_{ij}, d_{ijkl}\}$ are the coefficients of the corresponding effects.

The last pair of terms in $F_{\text{coup grad}}$ is possible to be excluded from the consideration assuming the insignificance of effects described by this summand. Variation of Eq. (1) in the $\{P, T, u_i\}$ variables gives us:

$$E_i = a_i P_i + \frac{a_{ij}}{2} P_i P_j^2 + \frac{a_{ijk}}{3} P_i P_j^2 P_k^2 + e_{kli} \varepsilon_{kl} + e_{kji} \varepsilon_{ij} P_i - g_{ijkl} D_{k,lj} + b_{ij} T_{,j} + f_{ijkl} \varepsilon_{jk,l}. \quad (7)$$

It should be noted that there is no summation over i in Eq. (7).

$$(\lambda_{ij} T_{,j})_i - t_{ij} \varepsilon_{ij} + a_{i0} P_i^2 / 2 + b_{ij} P_{i,j} - f_{ijk} \varepsilon_{ij,k} = 0 \quad (8)$$

$$\sigma_{ij} = c_{ijkl} \varepsilon_{kl} - (T - T_0) t_{ij} - e_{ijk} P_k - e_{ijk} P_k P_i. \quad (9)$$

Eqs. (7)–(9) should be supplemented by the standard boundary conditions at the interface:

$$T_1 = T_2; \lambda_{ij}^{(1)} T_{1,j} n_i = \lambda_{ij}^{(2)} T_{2,j} n_i; D_i^{(1)} n_i = D_i^{(2)} n_i; u_i^{(1)} = u_i^{(2)}; \sigma_{ij}^{(1)} n_j = \sigma_{ij}^{(2)} n_j, \quad (10)$$

which implies the continuity of the temperature, the heat flux, the deformation vector, the normal component of electric displacement, and the stress tensor. The indices 1 and 2 in Eq. (10) indicate the value location with respect to the number of the considered media; n_i are components of the vector normal to the boundary. At the outer boundary it is possible to assume temperature $T = T_0$ and heat flow $\lambda_{ij} T_{,j} n_i = q_0$ or their linear combination $\lambda_{ij} T_{,j} n_i + H_0 (T - T_0) = 0$. Here, q_0 is the heat flow at the boundary and H_0 is the heat transfer coefficient.

The mechanical boundary conditions can consist of the setting $\sigma_{ij} n_j = F_i$ and the displacement $u_i = P_i$, or have a mixed form, where $\{F_i, P_i\}$ are the components of forces and displacements at the boundary. The interface potential or the electrical intensity $E_i n_i = E_0$ can be used as the electrical boundary conditions. Note that it is also possible to consider a combination of the aforementioned quantities (impedance type boundary condition).

III. Thermoelastoelectric Potentials for Transversely Isotropic Medium

Due to the nonlinearity of Eq. (7), the solution of the problem described above is possible to obtain only numerically. Therefore, to derive analytical expressions describing the electric field distribution, we linearize Eq. (7) and consider a transversely isotropic medium. In this case the mechanical, dielectric, and piezoelectric properties of the ferroelectric are determined by a set of five modules of elasticity (c_{11} , c_{12} , c_{13} , c_{33} , c_{44}), two dielectric constants (κ_{11} , κ_{33}), and three piezomoduli (e_{31} , e_{33} , e_{15}).

The equilibrium equations, in terms of the stress σ_{ij} and the electric displacement D_i , are given by:

$$\sigma_{ij,j} = 0, D_{i,i} = 0, \quad i, j = 1, 2, 3. \quad (11)$$

The constitutive equations take the form:

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl} - e_{kij}E_k - t_{ii}(T - T_0), D_k = e_{kij}\varepsilon_{ij} + \varepsilon_0\kappa_{kl}E_l + P_{Sk}, \quad (12)$$

where \vec{P}_S is spontaneous polarization.

Let the (r, θ) be the plane of the cylindrical coordinate system (r, θ, z) , which coincides with the isotropic plane of the transversely isotropic medium. The poling direction is to be along the z -axis. The displacements and the electric potential may be expressed by the five potential functions U_i ($i = 1, 2, 3, 4, 5$) [9, 10]:

$$u_r = \sum_{i=1}^4 \frac{\partial U_i}{\partial r} - \frac{1}{r} \frac{\partial U_5}{\partial \theta}, \quad u_\theta = \sum_{i=1}^4 \frac{1}{r} \frac{\partial U_i}{\partial \theta} + \frac{\partial U_5}{\partial r}, \quad u_z = \sum_{i=1}^4 m_{1i} \frac{\partial U_i}{\partial z},$$

$$\varphi = \sum_{i=1}^3 m_{2i} \frac{\partial U_i}{\partial z}, \quad m_5 T = \frac{\partial^2 U_5}{\partial z^2}. \quad (13)$$

The constants $\{m_{14}, m_5\}$ are defined by the relations:

$$m_{14} = \frac{t_{33}(c_{44} - s_4 c_{11}) + t_{11}(c_{13} + c_{44})}{t_{11}(c_{33} - s_4 c_{44}) - t_{33}(c_{13} + c_{44})}, \quad s_4 = \frac{\lambda_{33}}{\lambda_{11}}, \quad m_5 = \frac{t_{11}}{c_{44} + (c_{13} + c_{44})m_{14} - c_{11}s_4}. \quad (14)$$

The remaining unknown constants m_1 and m_2 are defined below. Putting Eq. (13) into Eqs. (11), (12) yields:

$$\frac{\partial^2 U_i}{\partial r^2} + \frac{1}{r} \frac{\partial U_i}{\partial r} + \frac{1}{r^2} \frac{\partial^2 U_i}{\partial \theta^2} + \frac{\partial^2 U_i}{\partial z_i^2} = 0 \quad i = 1, \dots, 5, \quad (15)$$

where $z_i = z/\sqrt{s_i}$, s_4 is defined above, $s_5 = \frac{c_{44}}{c_{11} - c_{12}}$ and the other three roots s_i ($i = 1, 2, 3$) are determined from the characteristic equation:

$$As^3 + Bs^2 + Cs + D = 0. \quad (16)$$

In Eq. (16), the constants A, B, C, and D are the combinations of the material constants and given by:

$$A = c_{11}(e_{15}^2 + c_{44}\kappa_{11})$$

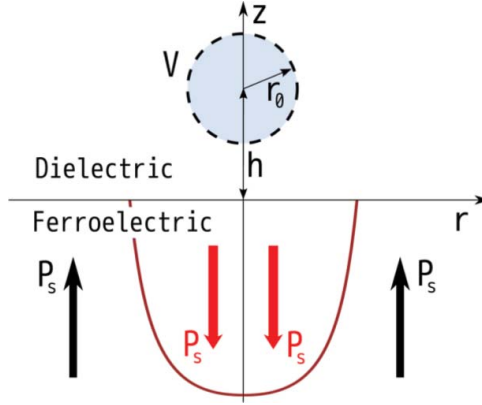


Figure 1. The configuration of the system under consideration. (Color figure available online).

$$\begin{aligned}
 B &= 2e_{15}(e_{15}c_{13} - e_{33}c_{11}) + 2c_{13}(e_{15}c_{31} + c_{44}\kappa_{11}) - c_{44}(e_{31}^2 + c_{11}\kappa_{33}) \\
 &\quad + \kappa_{11}(c_{13}^2 - c_{11}c_{33}), \\
 C &= e_{33}(e_{33}c_{11} + 2e_{15}c_{44}) - 2e_{33}(e_{15} + e_{31})(c_{13} + c_{44}) - \kappa_{33}(c_{13}^2 + 2c_{13}c_{44} - c_{11}c_{33}), \\
 &\quad + \kappa_{11}c_{33}c_{44} + c_{33}(e_{15} + e_{31})^2, \\
 D &= -c_{44}(e_{33}^2 + c_{33}\kappa_{33}). \tag{17}
 \end{aligned}$$

In Eq. (13) m_{1i} and m_{2i} ($i = 1, 2, 3$) are constants related to s_i by:

$$\begin{aligned}
 \frac{c_{44} + (c_{13} + c_{44})m_{1i} + (e_{15} + e_{31})m_{2i}}{c_{11}} &= \frac{c_{33}m_{1i} + e_{33}m_{2i}}{c_{13} + c_{44} + c_{44}m_{1i} + e_{15}m_{2i}} \\
 &= \frac{e_{13}m_{1i} - \kappa_{33}m_{2i}}{e_{15} + e_{31} + e_{15}m_{1i} - m_{2i}\kappa_{11}}. \tag{18}
 \end{aligned}$$

Thus, the displacements, the electric potential, and the temperature are expressed in terms of five potentials in sufficiently simple way. These potentials are solutions of the generalized Laplace Eq. (15). This approach allows us to obtain precise analytical expressions for certain problems of the thermopiezoelectric elasticity.

IV. Impact of the Piezoelectric Properties on Electric Field for SPM Tip

To illustrate the model described above, we consider the problem of calculating the electrostatic and elastic fields generated by a sphere of radius r_0 , which is maintained at a potential V (Fig. 1). The sphere is located in the upper (dielectric) half space at the height h . The lower half space is a both ferroelectric and piezoelectric. The problem is axisymmetric and, in addition, we assume uniform temperature distribution. In this case we can confine ourselves to the three potentials $\{U_1, U_2, U_3\}$ in ferroelectrics and the electrostatic potential φ_d in dielectric, which are the solutions of Eq. (15). To simplify subsequent calculations, as a new potentials we take derivatives with respect to z from the old ones. Additionally, let us introduce a new set of constants:

$$\mu_i = c_{44} + c_{44}m_{1i} + e_{15}m_{2i}$$

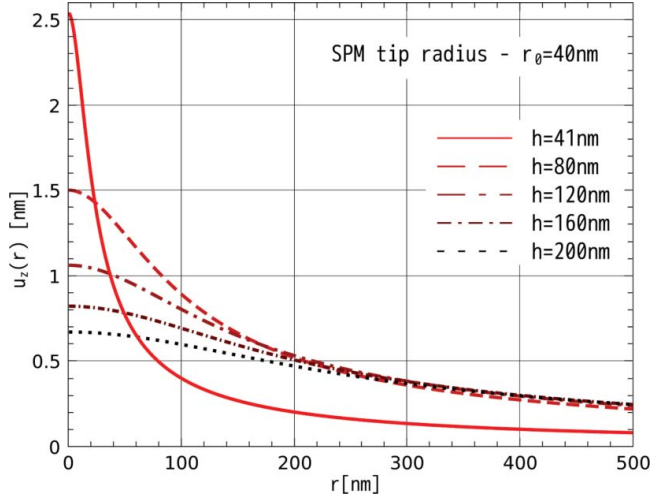


Figure 2. The coordinate dependence of the displacement vector vertical component for the different positions of the SPM tip. (Color figure available online).

$$v_i = s_i(e_{15} + e_{15}m_{1i} - \kappa_{11}m_{2i}). \quad (19)$$

Using these constants it is easy to write down the values that must be continuous at the boundary $z = 0$:

$$\varphi_d = \sum_{i=1}^3 m_{2i}U_i, \quad \sigma_{zz} = \sum_{i=1}^3 s_i\mu_i \frac{\partial U_i}{\partial z}, \quad \sigma_{zr} = \sum_{i=1}^3 \mu_i \frac{\partial U_i}{\partial r}, \quad D_z = \sum_{i=1}^3 v_i \frac{\partial U_i}{\partial z}. \quad (20)$$

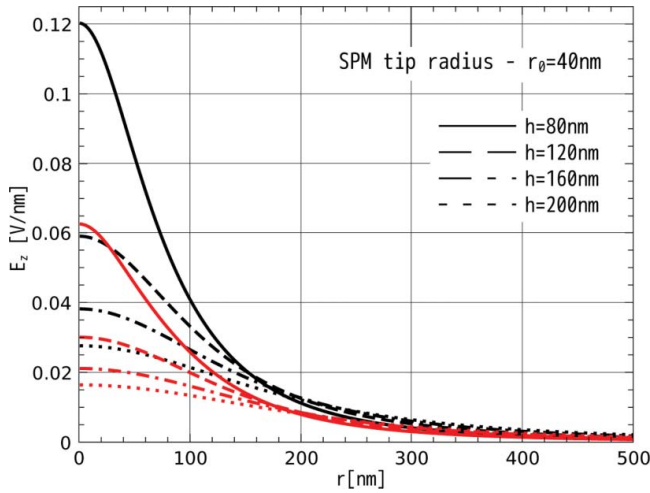


Figure 3. The coordinate dependence of the electric intensity vertical component on the SPM tip position with (thick red lines) and without (thin black lines) consideration of the piezoelectric properties of ferroelectric.

To solve problem (20) we shall use the bispherical coordinates associated with the initial cylindrical ones by the relations [11]:

$$r = \frac{c \sin \alpha}{\cosh \beta - \cos \alpha}, \quad z = \frac{c \sin \beta}{\cosh \beta - \cos \alpha}. \quad (21)$$

where, $c = \sqrt{h^2 - r_0^2}$ is the scale factor. The surface of the sphere and the boundary between the media are given by equations: $\beta = \beta_0$, $\cosh \beta_0 = h/r_0$, and $\beta = 0$, respectively. Solutions of Laplace's Eq. (15) are sought in the form of Fourier series:

$$U_i = V(\alpha, \beta) \sum_{n=1}^{\infty} U_{in} P_n(\cos \alpha) e^{-(n+1/2)\beta},$$

$$\varphi_d = V(\alpha, \beta) \sum_{n=1}^{\infty} (\varphi_{n1} \cosh(n + 1/2)\beta + \varphi_{n2} \sinh(n + 1/2)\beta) P_n(\cos \alpha), \quad (22)$$

where $V(\alpha, \beta) = V \sqrt{2(\cosh \beta - \cos \alpha)}$ and $P_n(\chi)$ is a Legendre polynomial.

The Fourier coefficients $\{U_{n1}, U_{n2}, U_{n3}\}$ are uniquely determined by substitution of Eq. (22) into the boundary conditions arising from the equations $\sigma_{zz} = \sigma_{zx} = 0$ - i.e. the continuity of the electrostatic potential and the normal component of the electric displacement at the interface and the specified value of the potential φ_d on the sphere. For the results visualization, solution of Eq. (22) was performed for PZT-4 ceramics. The coordinate dependence of the displacement vector vertical component for the different position of the scanning probe microscope (SPM) tip – sphere, is demonstrated in Figure 2. Additionally, in Figure 3 one can see the coordinate dependence of the electric intensity vertical component on the SPM tip position with/without (black lines) consideration of the piezoelectric properties of ferroelectric. It should be mentioned that a more accurate formula for this model can be obtained by taking into consideration the influence of the domain walls and the surface charge density at $z = 0$.

V. Conclusion

Basic physical ideas supported by precise calculations how to model the ferroelectric domain wall motion have been presented. The results obtained for PZT-4 ceramics employing the proposed theoretical approach have shown that the presence of the piezoelectric properties of a ferroelectric results in a significant reduction of the electric field. Moreover, we have demonstrated that for the proper description of domain wall motion it is necessary to take into account temperature, elastic stress, and electric displacement gradients. In this case the joint description of the thermal, electrical, and elastic phenomena is significantly simplified by the introduction of five potential functions. Our study may provide a theoretical basis and physical insights for the further domain wall motion phenomena investigations.

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