The Effect of Surface Inhomogeneity on Coupled Fields in Thermoelastic Polarized Small Scale Structures

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Acknowledgement. The author acknowledges support from the Slovak Research and Development Agency registered under number SK-CN-RD-18-0005.

Theoretical Background for Linear Local Gradient Electro-Thermo-Elasticity

The classical continuum theory does not reflect material microstructure and cannot be apply to study the small-scale structures. To overcome intrinsic limitations of classical theory of continua, the gradient-type models can be applied for investigation of micro-scale phenomena in materials. In the proposed work, the relations of the local gradient piezoelectricity are used to study the behavior of elastic small-scale solids (nanosize plates and fibers with free and clamped surfaces). The fundamentals of local gradient theory of dielectrics were developed in a series of papers and were generalized in the book [Hrytsyna O., Kondrat V. Local Gradient Theory for Dielectrics: Fundamentals and Applications. Jenny Stanford Publishing Pte Ltd, Singapore, 2020]. This theory is based on the consideration of coupling between the processes of mechanical deformations, thermal conductivity and polarization with the local mass displacements. The local mass displacement is linked to the microstructure ordering of the material including atomic arrangements (reordering) at the surface/interface regions.

The **purpose** of this work is

(*i*) Making use of the local gradient theory of dielectrics to derive the fundamental solutions to the wave equations for the infinite continuum and present Green's functions for the displacement and polarization vectors, the temperature field and modified chemical potential resulting from the action of concentrated body force, electric force, charge density and heat supply functions, all varying harmonically with time;

(*ii*) to test the relations of local gradient electro-thermo-elasticity on the simple boundary value problems and to study the effect of near-surface inhomogeneity on the coupled fields in nano-size piezoelectric plates and fibers with free and clamped surfaces.

Within the local gradient electro-thermo-electricity, the system of basic linear equations includes:

Field equations
$$\sigma_{ij,j}+\rho_0 F_i=\rho_0\ddot{}\qquad \rho_0 T_0\dot{}\qquad +\rho_0\mathfrak{R},\quad D_{i,i}=\rho_e,\quad \pi_{mi,i}+\rho_m=0 \qquad (1)$$

Constitutive relations
$$\sigma_{ij}=\rho_0\frac{\partial f}{\partial\varepsilon_{ij}},\quad s=-\frac{\partial f}{\partial T},\quad \pi_{ei}=-\frac{\partial f}{\partial E_i},\quad \rho_m=-\frac{\partial f}{\partial\mu'_\pi},\quad \pi_{mi}=\frac{\partial f}{\partial\mu'_{\pi,i}} \qquad (2)$$
$$D_i=\varepsilon_0 E_i+\rho_0\pi_{ei} \qquad (3)$$

Kinematic relations
$$\varepsilon_{ij}=\frac{1}{2}\left(u_{i,j}+u_{j,i}\right),\qquad q_i=-\lambda_{ij}T_{,j},\qquad E_i=-\varphi_{e,i} \qquad (4)$$

Here, $\hat{\boldsymbol{\sigma}}$ and $\hat{\boldsymbol{\varepsilon}}$ are the stress and strain tensors; $\mathbf{u}$ is the displacement vector; $\mathbf{F}$ denotes the mechanical mass force; ρ_0 is the mass density; ρ_e and ρ_m are the specific densities of the induced charge and induced mass, respectively; $\mathbf{D}$ represents the electric displacement vector; $\mathbf{E}$ and $\boldsymbol{\pi}_e$ are electric field and polarization vectors, respectively; φ_e is the electric potential; $\mu'_\pi=\mu_\pi-\mu$; μ is the chemical potential; μ_π is the energy measure of the effect of the local mass displacement on the internal energy; $\boldsymbol{\pi}_m$ is the specific vector of the local mass displacement; *T* is the temperature; *s* is the specific entropy; $\mathbf{q}$ is the heat flux vector; $f\left(\hat{\boldsymbol{\varepsilon}},T,\mathbf{E},\mu'_\pi,\nabla\mu'_\pi\right)$ is the generalized free energy; ε_0 is the permittivity of vacuum.

Formulation of the Boundary-Value Problems

Surface effect in piezoelectric nano-size plates and fibers with free and clamped surfaces

Task 1. Nano-size plate with clamped surfaces
$$x=h:\ u_x=0,\ \theta=\theta_1,\ \varphi_e=V,\ \bar{\mu}'_\pi(x)=\mu_{\pi a}$$
$$x=-h:\ u_x=0,\ \theta=\theta_2,\ \varphi_e=-V,\ \bar{\mu}'_\pi(x)=\mu_{\pi a}$$

Task 2. Nano-size plate with free upper surface and clamped bottom surface
$$x=h:\ \sigma_{xx}=0,\ \theta=\theta_1,\ \varphi_e=V,\ \bar{\mu}'_\pi(x)=-\mu_{\pi 0}$$
$$x=-h:\ u_x=0,\ \theta=\theta_2,\ \varphi_e=-V,\ \bar{\mu}'_\pi(x)=\mu_{\pi a}$$

Task 3. Nano-size fiber with clamped surface
$$r=R:\ u_r=0,\ \theta=\theta_*,\ \varphi_e=V,\ \bar{\mu}'_\pi(x)=\mu_{\pi a}$$

$$\sigma_{rr}=-\bar{\gamma}_T\theta_*-\frac{2\alpha_m A}{C_{12}+2C_{44}}\left\{C_{44}\frac{I_1(\Lambda r)}{\Lambda r}+\left[C_{12}+C_{44}+M\left(C_{12}+2C_{44}\right)\right]\frac{I_1(\Lambda R)}{\Lambda R}\right\}$$

In the thick plates and fibers with clamped surfaces, the normal (radial) stresses σ_{xx} and σ_{rr} are negligibly small, but decreasing thickness of solids leads to an increase of the absolute magnitude of these stresses. As a result, these stresses cause disjoining pressure
$$p_{dis}=\frac{1}{2h}\int_{-h}^{h}\sigma_{xx}dx,\qquad p_{dis}=\frac{1}{R}\int_{0}^{R}r\sigma_{rr}dr$$

Piezoelectric medium under the action of harmonic loading $\mathbf{F}(\mathbf{r},t)=\bar{\mathbf{F}}(\mathbf{r})e^{-i\omega t}$

Let us decompose the displacement, mass force and electric field vectors as the sum of its potential and solenoidal components:
$$\bar{\mathbf{u}}=\nabla\varphi_u+\nabla\times\boldsymbol{\psi}_u,\ \nabla\cdot\boldsymbol{\psi}_u=\mathbf{0},$$
$$\bar{\mathbf{F}}=\nabla\Phi+\nabla\times\boldsymbol{\Psi},\ \nabla\cdot\boldsymbol{\Psi}=\mathbf{0},\quad \mathbf{E}=-\nabla\varphi_e-\nabla\times\mathbf{K} \qquad (5)$$

Using Eqs. (1)-(5) the following governing set of equations can be obtained for local gradient continuum
$$\left(\Delta+m_1^2\right)\left(\Delta+m_2^2\right)\varphi_u=\frac{\gamma_T}{C}(\Delta-a_0)\theta-\frac{1}{c_1^2}\left(\Delta-\lambda_E^2\right)\Phi+a_1\rho_e,$$
$$\left(\Delta+\frac{\omega^2}{c_2^2}\right)\boldsymbol{\psi}_u=-\frac{1}{c_2^2}\boldsymbol{\Psi},\qquad (\Delta+m_3)\theta=-\Theta,$$
$$\Delta\left(\Delta+m_1^2\right)\left(\Delta+m_2^2\right)\varphi_e=-\kappa_E a_2(\Delta+a_3)\Delta\theta+\rho_0 a_1\Delta\Delta\Phi-a_6(\Delta\Delta-a_7\Delta-a_8)\rho_e,$$
$$\left(\Delta+m_1^2\right)\left(\Delta+m_2^2\right)\bar{\mu}'_\pi=a_2(\Delta+a_3)\theta+a_4\left(\Delta+\frac{\omega^2}{c_1^2}\right)\rho_e-a_5\Delta\Phi$$

Let us consider $\mathbf{F}\neq 0,\ \rho_e=0,\ \theta=0$
$$\varphi_u(\mathbf{r})=\frac{1}{4\pi c_1^2\left(m_1^2-m_2^2\right)}\int_{(V)}\frac{\Phi(\mathbf{r}')}{R}\left[\left(m_1^2+\lambda_E^2\right)e^{im_1R}-\left(m_2^2+\lambda_E^2\right)e^{im_2R}\right]dV(\mathbf{r}'),$$
$$\varphi_e(\mathbf{r})=-\frac{a_5\,\kappa_E}{4\pi\left(m_1^2-m_2^2\right)}\int_{(V)}\frac{\Phi(\mathbf{r}')}{R}\left[m_1^2e^{im_1R}-m_2^2e^{im_2R}\right]dV(\mathbf{r}'),$$
Here, $R=\sqrt{(x_1-x_1')^2+(x_2-x_2')^2+(x_3-x_3')^2}$

Numerical Calculations

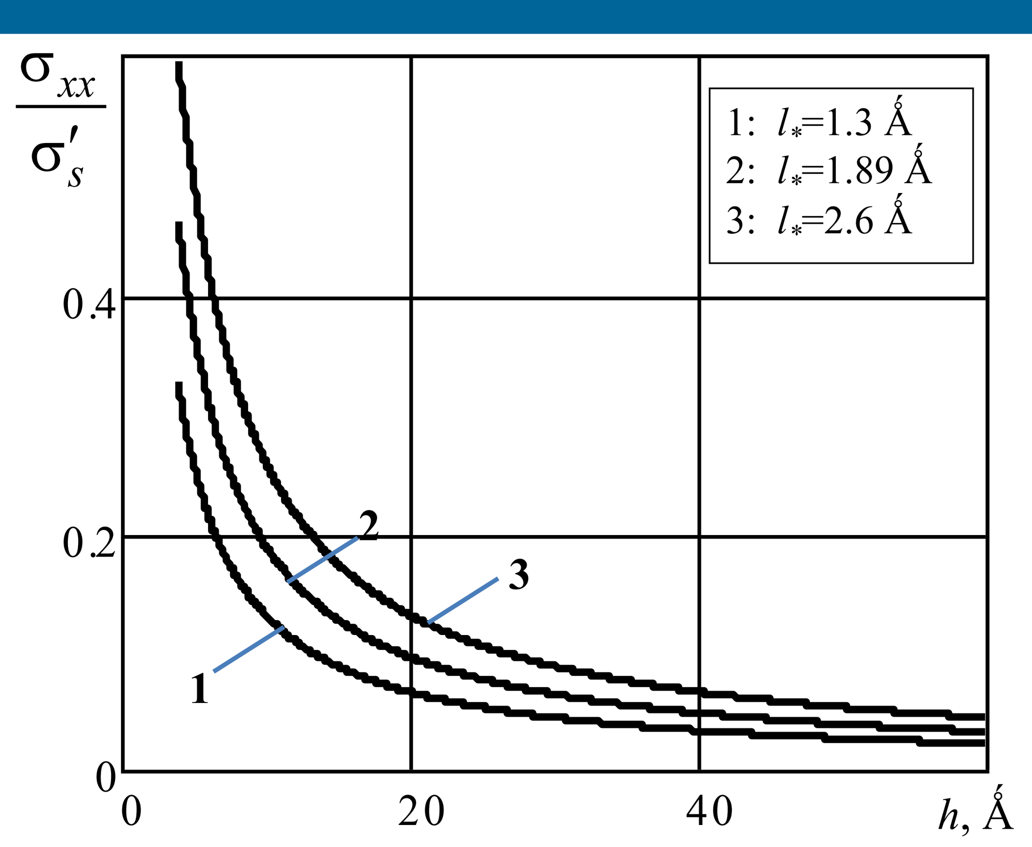

Figure 1. The dependence of the disjoining pressure on the film thickness for different materials (l_*= 1.3 Å, 1.89 Å, 2.6 Å, that is, curves 1–3, respectively)

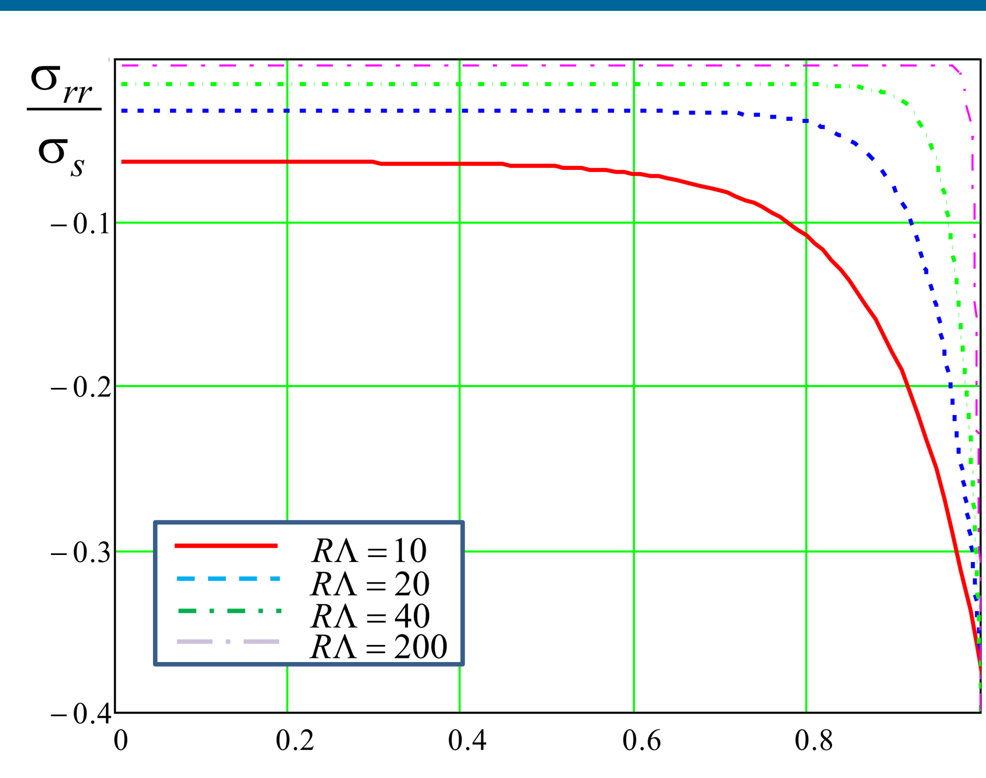

Figure 2. The distribution of radial stress in nano-size fibers of different radius (the coupling factor between the mechanical deformation and local mass displacement M = 0.01)

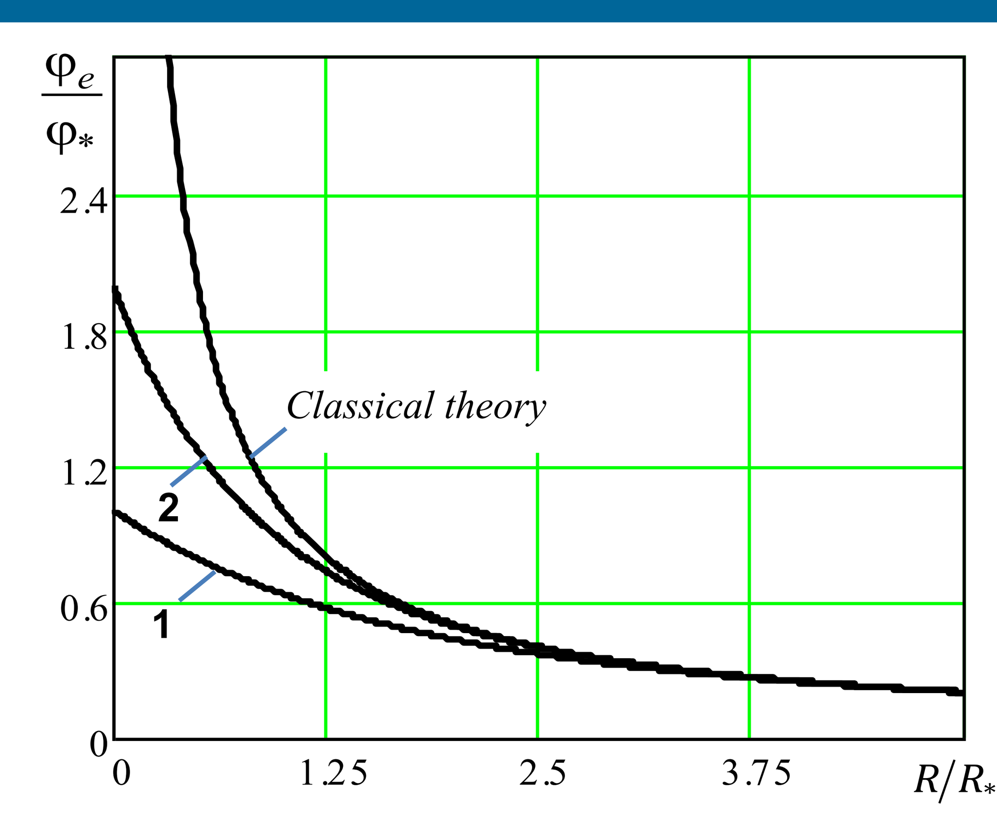

Figure 3. The dependence of the normalized potential field of a point electric charge on the dimensionless coordinate ($R_*/l_*=1$ and $R_*/l_*=2$, curves 1 and 2 respectively)

The main conclusions:

- By taking the local mass displacements into consideration the interaction between thermal, electric, and mechanical fields can be studied in polarized elastic continua including isotropic centrosymmetric materials with cubic symmetry.
- Within the local gradient theory of dielectrics, due to the changes in the material structure of near-surface regions the disjoining pressure appears in solid nano-thin layers and fibers, in which the regions of near-surface inhomogeneity overlap. If the thickness of small-scale structures diminishes, the disjoining pressure becomes higher.
- Within the local gradient theory the fundamental solutions to the wave equations for infinite piezoelectric continuum are derived. Expressions for the wave functions of the potentials of mechanical displacements vector as well as the electric potential and modified chemical potential are obtained for isotropic dielectrics subjected to the action of external harmonically varied with time loads. Using these solutions the Green functions for the temperature field, displacement and polarization vectors can be formulated.
- Contrary to the classical theory, the local gradient theory of dielectrics allows to avoid the singularity of the electric potential of a point charge in an infinite dielectric medium.
- The obtained analytical solutions to considered boundary-value problems could be useful to the design of new nanocomposite materials and small-scale devices as they provide new criteria for the prediction of size effects and electro-thermo-mechanical coupling in materials with high symmetry of the lattice.