Electro-Thermo-Mechanical Coupling in Isotropic Polarized Structures

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Theoretical Background for Linear Local Gradient Electro-Thermo-Elasticity

Classical piezoelectricity fails to explain the electro-thermo-mechanical coupling in centrosymmetric materials, as well as to cover both the surface and size effects in solids. To overcome intrinsic limitations of classical theory of dielectrics, the gradient-type models can be applied for investigation of micro-scale phenomena in materials. In this study, we used a local gradient theory of dielectrics which considers the interaction between the process of deformation of the body described by the displacement vector and the stress field, the electromagnetic processes characterized by the electromagnetic field vectors, the process of heat conduction characterized by the temperature field and the heat flux **q**, and the process of microstructure changes characterized by non-diffusive and non-convective mass flux (the local mass displacement - LMD). In this work, the relations of local gradient electro-thermo-elasticity are tested on the simple boundary value problem: the electro-thermo-mechanical coupling response of elastic dielectrics to the temperature gradients is studied.

The generalized free energy

$$f = f_0 - s_0\theta - \frac{C_V}{2T_0}\theta^2 + \frac{C_{12}}{2\rho_0}\varepsilon_{kk}\varepsilon_{nn} + \frac{C_{44}}{\rho_0}\varepsilon_{ij}\varepsilon_{ij} - \frac{\chi_E}{2}E_iE_i - \frac{d_\mu}{2}\bar{\mu}_\pi'^{\,2} - \frac{\chi_m}{2}\bar{\mu}'_{\pi,i}\bar{\mu}'_{\pi,i} - \frac{\gamma_T}{\rho_0}\theta\varepsilon_{kk} - \frac{\alpha_m}{\rho_0}\bar{\mu}'_\pi\varepsilon_{kk} - \beta_{T\mu}\theta\,\bar{\mu}'_\pi + \chi_{Em}E_i\bar{\mu}'_{\pi,i}$$

Within the local gradient electro-thermo-electricity, the system of basic linear equations includes [See, Hrytsyna O., Kondrat V. Local Gradient Theory for Dielectrics: Fundamentals and Applications. Singapore: Jenny Stanford Publishing Pte. Ltd., 2020]:

Field equations:

$$\sigma_{ij,j} + \rho_0F_i = \rho_0\ddot{u}_i,\quad \rho_0T_0\dot{s} = \lambda_{ij}\theta_{,ij} + \rho_0\Re,\quad \underbrace{D_{i,i} = \rho_e}_{\text{Gauss law}},\quad \underbrace{\pi_{mi,i} + \rho_m = 0}_{\text{balance equation for the induced mass}} \qquad (1)$$

Constitutive relations:

$$\sigma_{ij} = \rho_0\frac{\partial f}{\partial \varepsilon_{ij}},\quad s = -\frac{\partial f}{\partial \theta},\quad \pi_{ei} = -\frac{\partial f}{\partial E_i},\quad \rho_m = -\frac{\partial f}{\partial \mu'_\pi},\quad \pi_{mi} = \frac{\partial f}{\partial \mu'_{\pi,i}} \qquad (2)$$

$$D_i = \varepsilon_0E_i + \rho_0\pi_{ei} \qquad (3)$$

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, σ and ε 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; $\theta = T - T_0$, s is the specific entropy; $\mathbf{q}$ is the heat flux vector; $f\left(\varepsilon, \theta, \mathbf{E}, \mu'_\pi, \nabla\mu'_\pi\right)$ is the generalized free energy; ε_0 is the permittivity of vacuum.

Formulation of the Boundary-Value Problems

Coupled electro-elastic fields in isotropic dielectrics with a plane thermal inclusion

Consider an infinite plane isotropic (non-piezoelectric) layer of the thickness $2h$. The layer is in contact with two homogeneous half-spaces (Fig. 1). The body force and heat sources in the structure are not incorporated. The layer and the outside space are held at constant, but different temperature.

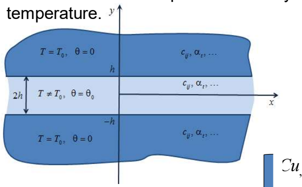

Figure 1. Infinite polarized medium with a plane thermal inclusion

Prescribed temperature distribution (thermal inclusion) in elastic dielectric medium:

$$\theta(y) = \theta_*\left[H(y+h) - H(y-h)\right] = \theta_*\begin{cases}0, & y \le -h\\ 1, & -h \le y \le h\\ 0, & y \ge h\end{cases} \qquad (5)$$

$$Cu_{,yy} - \alpha_m\bar{\mu}'_{\pi,y} = \gamma_T\,\theta_*\left[\delta(y+h) - \delta(y-h)\right] \qquad (6)$$

$$\bar{\mu}'_{\pi,yy} - \lambda_E^2\bar{\mu}'_\pi - \frac{\lambda_E^2\alpha_m}{\rho_0 d_\mu}u_{,y} = \eta\theta_*\left[H(y+h) - H(y-h)\right] \qquad (7)$$

$$E_{,y} - \kappa_E^2\bar{\mu}'_{\pi,yy} = 0 \qquad (8)$$

At both interfaces $y = \pm h$ all fields should be continuous:

$$\left[u_y\right]_{y=\pm h} = 0,\ \left[\sigma_{yy}\right]_{y=\pm h} = 0,\quad \left[E_y\right]_{y=\pm h} = 0,\ \left[\bar{\mu}'_\pi\right]_{y=\pm h} = 0 \qquad (9)$$

At both infinities $y = \pm\infty$ all fields should be finite:

$$u \to const,\ E \to 0,\ \bar{\mu}'_\pi \to 0 \text{ at } y \to \pm\infty \qquad (10)$$

	Mechanical displacement	Electric field
Local gradient theory	$u = u_*\begin{cases}-h + \Omega e^{y/l_*}\sinh(h/l_*), & y \le -h\\ y - \Omega e^{-h/l_*}\sinh(y/l_*), & -h \le y \le h\\ h - \Omega e^{-y/l_*}\sinh(h/l_*), & y \ge h\end{cases}$	$E = E_*\begin{cases}-e^{y/l_*}\sinh(h/l_*), & y \le -h\\ e^{-h/l_*}\sinh(y/l_*), & -h \le y \le h\\ e^{-y/l_*}\sinh(h/l_*), & y \ge h\end{cases}$
Classical theory	$u_{cl} = \frac{\theta_*\gamma_T}{C}\begin{cases}-h, & y \le -h\\ y, & -h \le y \le h\\ h, & y \ge h\end{cases}$	$E_{cl} = 0$

$$\Omega = \frac{\beta_{T\mu} + \gamma_T\alpha_m/(\rho_0C)}{\Lambda\left(\beta_{T\mu} - \gamma_Td_\mu/\alpha_m\right)},\qquad l_* = \frac{1}{\Lambda},\qquad \Lambda^2 = \frac{d_\mu(1+\mathfrak{M})}{(\chi_m - \kappa_E\chi_{Em})},\qquad \mathfrak{M} = \frac{\alpha_m^2}{\rho_0d_\mu C}$$

In non-piezoelectric crystals, classical theory predicts the linear distribution of the mechanical displacement within the layer, displacements outside the layer should be homogeneous. Within the framework of the local gradient theory, the smooth profile for displacement field is obtained. Also, the medium outside the layer is now not free of distortions. In case of thick layers, the local gradient theory correction would scarcely be important for strain field. However, if the thickness of the layer diminishes and becomes comparable to the material microstructural characteristic length, the nonlinearity in distribution of the displacement increases. The nonlinear law of distribution of displacement is more pronounced for more narrow layers. As a consequence, the profile of mechanical displacement in the nano-thin elastic layer significantly deviates from the linear law predicted by the classical theory.

Numerical Calculations

The polarization of elastic solids induced by the temperature gradient is known as a **thermal polarization effect.** A temperature gradient breaks the inversion symmetry and induces polarization even in centrosymmetric materials. Classical theory fails to capture this effect in non-piezoelectric structures. The local gradient theory describes the thermal polarization effect in isotropic centrosymmetric materials with cubic symmetry. It is shown that in thermoelastic polarized layered structure, a part of the thermal energy induced by the non-uniform temperature distribution is spent on the body polarization.

$$\pi_e(y) = -\theta_*\frac{\varepsilon_0}{\varepsilon}\frac{\bar{\beta}_{T\mu}\chi_{Em}}{d_\mu l_*(1+\mathfrak{M})}\begin{cases}-\sinh(h/l_*)\exp(y/l_*), & y < -h,\\ \sinh(y/l_*)\exp(-h/l_*), & -h \le y \le h,\\ \sinh(h/l_*)\exp(-y/l_*), & y > h.\end{cases}$$

The density of the bound surface charge induced on the interfaces

$$\sigma_{es}(\pm h) = \rho_0\pi_e(\pm h) = \mp\frac{\theta_*\rho_0\bar{\beta}_{T\mu}\chi_{Em}}{d_\mu(1+\mathfrak{M})l_*}\frac{\varepsilon_0}{\varepsilon}\sinh(h/l_*)\exp(-h/l_*)$$

Thermal inclusion induced the electric polarization of interfaces and can excite rather high electric field in very narrow regions around the interfaces: $E_* \sim 10^4\left[V/m\right]$

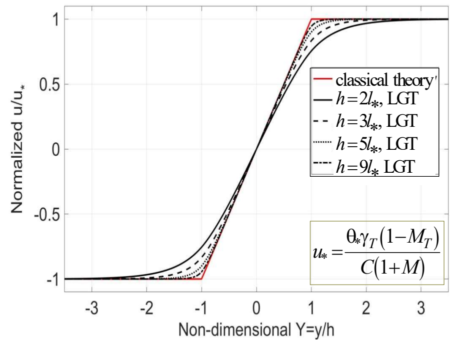

Figure 2. Distribution of the normalized displacement u/u_* caused by the thermal inclusion in non-piezoelectric elastic structure.

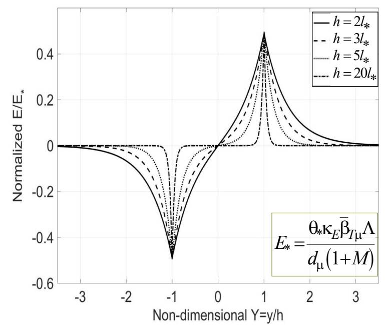

Figure 3. Distribution of the electric field E/E_* induced by the thermal inclusion in non-piezoelectric elastic structure.

The main conclusions:

The stationary electric and mechanical fields induced by the prescribed temperature distributions in polarized isotropic (non-piezoelectric) layered structures are studied. To this end, the local gradient theory of dielectrics is used. It is found that the distribution of mechanical displacement in narrow layer with thermal inclusion may be significantly changed with respect to the ones predicted by the classical solution. This phenomenon is size-dependent and it can be neglected by increasing the size of thermal inclusion. The introduction of the local mass displacement parameters into governing equations makes the distribution of displacement smooth. Moreover, the plane thermal inclusion in non-piezoelectric structure induces the electric field and polarization localized close to the thermal inclusion interfaces. Due to the layer polarization, the bound electric charges are induced on the layer interfaces. Hence, the thin thermal inclusion produces the thermal polarization effect and impacts the distribution of coupled physical fields in the vicinity of the thermal inclusion interfaces.

The local gradient theory of dielectrics provides a basis for the investigation of **micro-scale effect and electro-thermo-mechanical coupling phenomena in materials of arbitrary symmetry**, including the isotropic centrosymmetric crystals. The theory should be potentially helpful in some practical applications where the size effect is used. The local gradient theory of dielectrics can also contribute to the development of novel electro-thermo-mechanical coupling devices where the large temperature gradient may occur.