Effect of Local Mass Displacement on Coupled Fields in Dielectric Nano-Beam

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Field

Theoretical Background for Local Gradient Theory of Dielectrics

The **purpose** of this work is

- (i) to derive a general formulation of the linear local gradient electroelasticity by variational principle,
- (ii) to establish a local gradient Bernoulli-Euler dielectric beam model, and
- (iii) to test the obtained relations on the simple problem of a cantilevered piezoelectric beam under the end-point loading.

We consider an elastic polarized nonferromagnetic body that occupies the domain (V) and is bounded by a smooth surface. Let the body be under the effect of external forces and electric field inducing mechanical and polarization processes in it. To describe a more complex material behavior, local gradient theory of dielectrics takes into account the changes in the material microstructure alongside the mechanical deformation and electric polarization. This theory relates the above microstructure changes to the process of the local mass displacement (see for details Hrytsyna, O, and Kondrat, V. Local Gradient Theory for Dielectrics: Fundamentals and Applications. Jenny Stanford Publishing Pte. Ltd., 2020).

$$\delta \left[-\int_{(V_*)} H \, dV + \int_{(V)} W_V \, dV + \int_{(\Sigma)} W_s \, d\Sigma \right] = 0$$

the virtual work done by the external body force and surface loading

For the linear stationary isothermal approximation, the system of basic equations includes:

Constitutive relations $\nabla \cdot \hat{\boldsymbol{\sigma}} + \rho_0 \mathbf{F} = 0, \quad \nabla \cdot \mathbf{D} = \rho_e, \quad \nabla \cdot \boldsymbol{\pi}_m + \rho_m = 0$

equations

 $\hat{\boldsymbol{\sigma}} = \rho_0 \frac{\partial u}{\partial \hat{\boldsymbol{\varepsilon}}} \Big|_{\boldsymbol{\pi}_e, \boldsymbol{\pi}_m, \rho_m} \mathbf{E} = \frac{\partial u}{\partial \boldsymbol{\pi}_e} \Big|_{\hat{\boldsymbol{\varepsilon}}, \boldsymbol{\pi}_m, \rho_m} \boldsymbol{\mu}_{\boldsymbol{\pi}}' = \frac{\partial u}{\partial \rho_m} \Big|_{\hat{\boldsymbol{\varepsilon}}, \boldsymbol{\pi}_m, \boldsymbol{\pi}} \nabla \boldsymbol{\mu}_{\boldsymbol{\pi}}' = -\frac{\partial u}{\partial \boldsymbol{\pi}_m} \Big|_{\hat{\boldsymbol{\varepsilon}}}$

 $\mathbf{D} = \varepsilon_0 \mathbf{E} + \rho_0 \boldsymbol{\pi}_e$

Kinematic relations

$$\hat{\boldsymbol{\varepsilon}} = \frac{1}{2} \left[\boldsymbol{\nabla} \otimes \boldsymbol{u} + \left(\boldsymbol{\nabla} \otimes \boldsymbol{u} \right)^{\mathrm{T}} \right] \quad \boldsymbol{E} = -\boldsymbol{\nabla} \boldsymbol{\varphi}$$

Here, $\hat{\sigma}$ and $\hat{\epsilon}$ are the stress and strain tensors; **u** is the displacement vector; **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; D represents the electric displacement vector; E and π_{e} are electric field and polarization vectors, respectively; ϕ 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; π_m is the specific vector of the local mass displacement; $u(\hat{\boldsymbol{\varepsilon}}, \boldsymbol{\pi}_e, \rho_m, \boldsymbol{\pi}_m)$ is the generalized internal energy; ε_0 is the permittivity of vacuum.

 $H(\hat{\boldsymbol{\varepsilon}}, \mathbf{E}, \tilde{\boldsymbol{\mu}}'_{\pi}, \nabla \tilde{\boldsymbol{\mu}}'_{\pi}) = u - \mathbf{E} \cdot \boldsymbol{\pi}_{e} - \boldsymbol{\mu}'_{\pi} \rho_{m} + \nabla \boldsymbol{\mu}'_{\pi} \cdot \boldsymbol{\pi}_{m} - \frac{\varepsilon_{0}}{2\rho_{0}} \mathbf{E} \cdot \mathbf{E} \quad \text{is the generalized electric enthalpy}$

Bernoulli-Euler Local Gradient Dielectric Beam Model

In a state of plane strain, gradient-type constitutive relations are

$$\begin{split} \sigma_{11} &= C_{11}\varepsilon_{11} + C_{13}\varepsilon_{33} - e_{31}E_3 - \alpha_1^{\mu}\tilde{\mu}'_{\pi}, \\ \sigma_{33} &= C_{13}\varepsilon_{11} + C_{33}\varepsilon_{33} - e_{33}E_3 - \alpha_3^{\mu}\tilde{\mu}'_{\pi}, \\ \sigma_{31} &= 2C_{55}\varepsilon_{31} - e_{15}E_1, \quad \rho_m = d_{\mu}\tilde{\mu}'_{\pi} + \rho_0^{-1} \left(\alpha_1^{\mu}\varepsilon_{11} + \alpha_3^{\mu}\varepsilon_{33}\right), \\ \pi_e^1 &= \chi_1^E E_1 + \frac{2}{\rho_0} e_{15}\varepsilon_{31}, \quad \pi_e^3 = \chi_3^E E_3 + \rho_0^{-1} \left(e_{31}\varepsilon_{11} + e_{33}\varepsilon_{33}\right), \\ \pi_m^1 &= -\chi_1^m \tilde{\mu}'_{\pi,x}, \qquad \pi_m^3 = -\chi_3^m \tilde{\mu}'_{\pi,z} \end{split}$$



Figure 1. The cantilever beam with rectangular cross section subjected to a tip-point load

Based on the gradient-type constitutive relations of the local gradient electromechanics, the stationary balance equations and corresponding boundary conditions for the cantilever piezoelectric beam subjected to the end-point loading are derived from the variational principle. In this case,

$$\delta \int_{(V)} H \, dV = \int_{(V)} \left(\frac{1}{\rho_0} \sigma_{11} \delta \varepsilon_{11} - \rho_m \, \delta \tilde{\mu}'_{\pi} + \pi_m^1 \, \delta \tilde{\mu}'_{\pi,x} + \pi_m^3 \, \delta \tilde{\mu}'_{\pi,z} \right) dV$$

The analytical solution is obtained assuming the plane strain state of a beam and Bernoulli-Euler kinematic hypothesis

 $u_1(x,z) = -zw_{,x}$ $u_2 = 0$, $u_3(x) = w(x)$, $\tilde{\mu}'_{\pi}(x,z) = zm(x)$.

In view of Gauss-Coulomb law

Governing equations are:

Here, $M = \int \int \sigma_{11} z dz dy$

 $D_{3,z} = 0 \implies E_3 = -\frac{e_{31}}{a_{33}}\varepsilon_{11}$ $\bar{C}_{11}w,_{xxxx}+\alpha_1^{\mu}m,_{xx}=0,$

$$m_{,xx} - \lambda_0^2 \left(1 + \mathfrak{M}_h\right) m + \frac{\alpha_1^\mu}{\rho_0 \chi_1^m} w_{,xx} = 0$$

For cantilever beam subjected to a tip-point load, the boundary conditions are: x = 0: w = 0, $w_{x} = 0$, m = 0

$$x = L: M = 0, M_{x} = Q, m = 0$$

Obtained analytical solution is used for the validation of the size-dependent behavior of piezoelectric nanocantilever beam.

Numerical Calculations for PZT-5H







Figure 2. Dielectric beam deflection with different coupling factor \mathfrak{M} between the mechanical fields and the local mass displacement. Comparison between the local gradient beam theory (LGBT), classical beam theory (CBT), and strain gradient beam theory (SGBT) of dielectrics

Length, nm

Figure 3. Variation of the end point beam deflection w(L) with the beam length L. Comparison between the classical beam theory, strain gradient beam theory, and local gradient theory of the beam

Figure 4. Variation of the end point beam deflection w(L) with the beam thickness *h*. Comparison between the strain gradient beam theory and local gradient beam theory

The main conclusions:

- Within the local gradient theory, the dielectric beam deflection is smaller than that in the classical Bernoulli-Euler dielectric beam model.
- This shows that the local mass displacement being taken into account stiffens the nanocantilever beam.
- Due to the piezoelectric effect, the deflection predicted by the local gradient theory of the dielectric beam is smaller than that provided by the classical theory of an elastic beam. The size effect induced by the local mass displacement is significant when the beam thickness is small and close to the material length scale parameter.
- In this case, the differences in the deflection values predicted by the local gradient dielectric beam model and classical beam model can be large.
- Such a result agrees well with experimental studies and Bernoulli-Euler strain gradient theory.
- In the case of neglecting the local mass displacement, the local gradient dielectric beam theory reduced to the classical beam theory.
- The developed local gradient model of dielectric beams may be used to design new devices that utilize the piezoelectric micro/nano-beam elements as constituting blocks.