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Size-dependent bending of an electro-elastic bilayer nanobeam due to flexoelectricity and strain gradient elastic effect

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ABSTRACT

A size-dependent bending model of an electro-elastic bilayer nanobeam including an isotropic dielectric layer and an elastic layer is established based on the flexoelectricity theory and the strain gradient theory. The governing equations and boundary conditions are derived from electric enthalpy variation principle with consideration of electrostatic force. The static bending problems of bilayer cantilever under closed and open circuit conditions are solved to show the size-dependency of the flexoelectric effect in both direct and converse flexoelectric processes. Numerical results demonstrate that both the strain gradient elastic effect and the flexoelectric effect significantly influence the deflection of the bending cantilever when the beam thickness is comparable to the material length scale parameters. Due to the flexoelectricity, sharp gradients of the electric field and polarization field arise near the surfaces, which differs greatly from the uniform field in the classical theory. In addition, the electric potential generated in the direct flexoelectric process and the deflection generated in the converse flexoelectric process exhibit obvious size-dependency.

1. Introduction

Flexoelectricity, the coupling between polarization and strain gradients, is a universal effect allowed by symmetry in all dielectrics [1,2]. Since strain gradient is closely related to the characteristic scale (thickness, radius, etc.) of structures, flexoelectricity has increasing influence on the electrical and mechanical properties of dielectrics with their structural size decreasing to nanometers. In literatures, for example, flexoelectricity was found to play an important role in the physical characteristics of ferroelectrics. Catalan et.al [3] found that the flexoelectricity causes an order-of–magnitude decrease in the dielectric constant of thin films. Lubomirsky et.al [4] reported that the poling of quasi-amorphous $BaTiO_3$ upon cooling is assisted by flexoelectricity. Based on these observations, flexoelectricity is believed to have a good application potential in the engineering field.

Recently, flexoelectricity has stimulated a surge of scientific interests in both experimental and theoretical investigations. Some experiments have been successfully performed to estimate the flexocoupling coefficients. For example, Cross and coworkers [5–7] used the cantilever bending method and the pyramid-compression method to measure the flexocoupling coefficient in some certain perovskite ceramics. Zubko et al. [8,9] employed the three-point bending method to measure the flexocoupling coefficient in nonpiezoelectric $SrTiO_3$ single crystals of different crystallographic orientations. In these experiments, giant flexocoupling coefficients are found in some titanate material whose dielectric constants are very high.

Besides, some theoretical studies have also been done to interpret flexoelectricity in dielectrics. Kogan [10] formulated the first phenomenological theory of flexoelectricity in 1964 and estimated the value range of flexoelectric coefficients. Mindlin [11] introduced first gradients of the polarization into the conventional linear electromechanical coupling theory based on the long-wavelength limit of the shell-model of lattice dynamics. Tagantsev [12] developed a microscopic theory of ionic flexoelectricity based on a rigid-ion model. The author verified that there are four mechanisms contributing to the flexoelectric response: dynamic bulk flexoelectricity, static bulk flexoelectricity, surface flexoelectricity and surface piezoelectricity. The first steps towards a microscopic description of the electronic contribution to flexoelectricity were made by Resta [13]. Sharma et al. [14,15] developed a theory considering first gradients of the strain and the polarization and analyzed the size-dependent mechanical and electrical behaviors of piezoelectric and nonpiezoelectric nanostructures based on a combination of theoretical and atomistic

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approaches. Then a more comprehensive theory with consideration of surface stress, surface polarization, bulk flexoelectric effect and electrostatic force for elastic dielectrics was proposed by Shen and Hu [16]. These theories have already been used to interpret or predict some size-dependent mechanical and electrical behaviors of nanosized dielectric structures.

In literatures, flexoelectric effects on the mechanical and electrical properties of specific nanosized structures have been analyzed based on these theories. Liang et al. [17] established a Bernoulli–Euler dielectric nanobeam model with the strain gradient elastic effect and the flexoelectric effect. In their paper the size-dependent mechanical behaviors of pure elastic, piezoelectric and nonpiezoelectric dielectric cantilever beams were discussed. Influence of the flexoelectric effect on the electroelastic and dynamic responses of bending piezoelectric nanobeams under different boundary conditions was also investigated by Yan and Jiang [18] based on Bernoulli–Euler beam model and Timoshenko beam model. Zhang et al. [19] proved that flexoelectricity has significant influence on the electroelastic responses and vibrational behaviors of a piezoelectric nanoplate. These researches mainly targeted at monolayer simple structures such as nanobeam and nanoplate.

Moreover, a bilayer or a multilayer structure is also widely used in mems-electro-mechanical system (MEMS) and nano-electro-mechanical system (NEMS) [20–23], such as a piezoelectric bimorph sensor [24]. Several analyses about the effect of flexoelectricity on bilayer or multilayer dielectric structures could be found. Sharma et al. [25] proved the possibility of creating apparently piezoelectric multilayer thin films by only symmetrically stacking various nonpiezoelectric dielectric materials with different dielectric constant. When the multilayer structure is subjected to a pressure, the large strain gradients induced near the interfaces will generate a net polarization. Chen and Soh [26] investigated the flexoelectric effects on the distributions of polarization in multiferroic electro-magnetic thin bilayer films. They found that the flexoelectric induced polarization became more and more dominant with the film thickness decreases. Li et al. [27] analyzed a three-layer beam structure including an isotropic dielectric layer, an electrode layer and an elastic substrate layer based on the extended linear piezoelectricity theory proposed by Hadjesfandiari [28]. Their analysis demonstrated that the size-dependent flexoelectricity significantly affects the static and dynamic behaviors of the three-layer bending beam. Besides, for bilayer or multilayer nanosized structures, the strain gradient elastic effect may play a key role in its mechanical properties. Such an effect on the composite structures has been widely investigated especially in recent years [29–33]. Analogous to the bilayer piezoelectric intelligent structure, a bilayer flexoelectric dielectric structure (including an isotropic dielectric layer and an elastic layer) may also possess exciting electrical and mechanical properties and have the possibility of the application in engineering. However, the investigation and application of such an electro-elastic bilayer structure is still absent. Further exploration of the flexoelectricity and strain gradient effect in such bilayer structures is necessary. This paper aims at performing some theoretical analyses of the flexoelectricity and strain gradient effect in nanosized bilayer flexoelectric beams.

In the present analysis, a size-dependent bending model of a bilayer flexoelectric dielectric nanobeam is proposed based on the Bernoulli–Euler beam model and the flexoelectricity theory with consideration of the effects of strain gradients and polarization gradients. The details are as follows: in Section 2, some basic equations in flexoelectric theory are given; in Section 3, the governing equations and boundary conditions of a bilayer flexoelectric dielectric nanobeam are derived; in Section 4, static bending problems of the bilayer cantilever under closed and open circuit conditions are solved. The new model can be used to illustrate the size-dependent flexoelectricity of a bilayer dielectric cantilever; in Section 5, numerical results are given to discuss the influence of strain gradient and flexoelectric effects on the mechanical and electrical properties. Finally, main conclusions for this paper are summarized in Section 6.

2. Basic equations in flexoelectric theory

For an extended linear theory of centrosymmetric dielectrics, the expression for the internal energy density U incorporating first gradients of the deformation gradient and the polarization is given in [34]. Another form of the internal energy density incorporating first gradients of the strain and the polarization can be written as

$$U = \frac{1}{2}a_{kl}P_kP_l + \frac{1}{2}c_{ijkl}\varepsilon_{ij}\varepsilon_{kl} + \frac{1}{2}b_{ijkl}P_{i,j}P_{k,l} + f_{ijkl}P_i\eta_{jkl} + d_{ijkl}P_{i,j}\varepsilon_{kl} + \frac{1}{2}g_{ijklmn}\eta_{ijk}\eta_{lmn}, \quad (1)$$

where $\mathbf{a}$ and $\mathbf{c}$ are the second-order reciprocal dielectric susceptibility and fourth-order elastic constant tensors, respectively. $\mathbf{d}$ and $\mathbf{f}$ are the flexocoupling coefficient tensors, and it was justified that $\mathbf{d} = -\mathbf{f}$ [16,35]. The tensor $\mathbf{g}$ represents strain gradient elastic effect. The summation convention is used in this paper, and the comma in the subscript indicates differentiation with respect to the spatial variables. $\mathbf{P}$ denotes the polarization vector. $\boldsymbol{\varepsilon}$ and $\boldsymbol{\eta}$ are the strain and strain gradient tensors, respectively, which are defined as,

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \eta_{ijk} = \varepsilon_{ij,k} = \frac{1}{2}(u_{i,jk} + u_{j,ik}). \quad (2)$$

Here $\mathbf{u}$ represents the displacement vector.

The electric enthalpy density is defined by Toupin [36] as

$$H = U - \frac{1}{2}\varepsilon_0\varphi_{,i}\varphi_{,i} + \varphi_{,i}P_i, \quad (3)$$

where ε_0 is the permittivity of vacuum and φ is the electric potential of the Maxwell self-field (MS) defined by

$$E_i^{MS} = -\varphi_{,i}. \quad (4)$$

The constitutive equations are expressed in terms of the internal energy as

$$\sigma_{ij} = \frac{\partial U}{\partial \varepsilon_{ij}} = c_{ijkl}\varepsilon_{kl} + d_{ijkl}P_{i,j}, \quad (5)$$

$$\tau_{ijk} = \frac{\partial U}{\partial \eta_{ijk}} = f_{ijkl}P_i + g_{ijklmn}\eta_{lmn}, \quad (6)$$

$$E_i = \frac{\partial U}{\partial P_i} = a_{ij}P_j + f_{ijkl}\eta_{jkl}, \quad (7)$$

$$X_{ij} = \frac{\partial U}{\partial P_{i,j}} = b_{ijkl}P_{k,l} + d_{ijkl}\varepsilon_{kl}. \quad (8)$$

In the above equations, $\boldsymbol{\sigma}$ is the classical Cauchy Stress tensor, $\boldsymbol{\tau}$ is the high-order stress tensor, $\mathbf{E}$ is the effective local electric field vector, $\mathbf{X}$ is the high-order local electric field. For an isotropic dielectric, the symmetries of the material constants introduced in Eq. (1) are as follows [34],

$$\begin{cases} a_{ij} = a\delta_{ij}, \quad c_{ijkl} = c_{12}\delta_{kl} + c_{44}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\ b_{ijkl} = b_{12}\delta_{kl} + b_{44}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + b_{77}(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}) \\ d_{ijkl} = d_{12}\delta_{kl} + d_{44}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\ f_{ijkl} = f_{12}\delta_{kl} + f_{44}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \end{cases}. \quad (9)$$

The coefficient tensor $\mathbf{g}$ corresponds to the adopted strain gradient elastic theory. The differences/similarities of various strain gradient theories have been investigated by Zhang and Sharma [37]. In this paper, the theory proposed by Kleinert and Gauge [38] is used. For an isotropic material, the elements of the coefficient tensor $\mathbf{g}$ can be derived as