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Size-dependent piezoelectricity

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ABSTRACT

In this paper, a consistent theory is developed for size-dependent piezoelectricity in dielectric solids. This theory shows that electric polarization can be generated as the result of coupling to the mean curvature tensor, unlike previous flexoelectric theories that postulate such couplings with other forms of curvature and more general strain gradient terms ignoring the possible couple-stresses. The present formulation represents an extension of recent work that establishes a consistent size-dependent theory for solid mechanics. Here by including scale-dependent measures in the energy equation, the general expressions for force- and couple-stresses, as well as electric displacement, are obtained. Next, the constitutive relations, the uniqueness theorem and the reciprocal theorem for the corresponding linear small deformation size-dependent piezoelectricity are developed. As with existing flexoelectric formulations, one finds that the piezoelectric effect can also exist in isotropic materials. However, in the present theory there is only one flexoelectric constant for isotropic material and the coupling is strictly through the skew-symmetric mean curvature tensor. In the last portion of the paper, this isotropic case is considered in detail by developing the corresponding boundary value problem for two dimensional analyses and obtaining a closed form solution for an isotropic dielectric cylinder.

1. Introduction

Recent developments in micromechanics, nanomechanics and nanotechnology require advanced size dependent electromechanical modeling of coupled phenomena, such as piezoelectricity. Classical piezoelectricity describes the relation between electric polarization and strain in non-centrosymmetric dielectrics at the macro-scale (Cady, 1964). However, some experiments have reported about size-effect phenomena of piezoelectric solids and linear electromechanical coupling in isotropic materials (Mishima et al., 1997; Shvartsman et al., 2002; Buhlmann et al., 2002; Cross, 2006; Harden et al., 2006; Zhu et al., 2006; Baskaran et al., 2011; Catalan et al., 2011). The classical theory cannot address this size dependency, because it considers that matter is continuously distributed throughout the body by neglecting its microstructure. Therefore, it is necessary to develop a size-dependent piezoelectricity, which accounts for the microstructure of the material by introducing higher gradient of deformation. Wang et al. (2004) have developed a size-dependent piezoelectric theory by considering the rotation gradient effect in the framework of the couple stress theory. In this formulation the electric polarization is related to the macroscopic rotation gradient. However, the theory suffers from its dependence on an underlying inconsistent couple stress theory. In some circles this size-dependent character for linear response is known as the flexoelectric effect (Kogan, 1964; Meyer, 1969), where the dielectric polarization is related to the macroscopic strain gradient or curvature strain. This theory predicts that in principle the flexoelectric effect is nonzero for all dielectrics, including the isotropic ones. Although there are some developments in this direction (Tagantsev, 1986; Maranganti et al., 2006; Eliseev et al., 2009), these theories also suffer from the use of different inconsistent second order gradients of deformation, as well as ignoring the possible couple-stress effect. There have been some experimental studies, which correlate their data with these theories (e.g., Cross, 2006; Harden et al., 2006; Zhu et al., 2006; Zubko et al., 2007; Baskaran et al., 2011; Catalan et al., 2011; Morozovska et al., 2012). It should also be mentioned that the surface effects (e.g., residual surface stress, surface elasticity) have often been adopted to analyze the size effects. For example, Pan et al. (2011) established a continuum theory of surface piezoelectricity for dielectric materials. However, it seems there is a relation between the continuum size-dependent piezoelectricity theory and the continuum theory of surface piezoelectricity, which needs further development.

Thus, the first step toward developing consistent size-dependent electromechanical theories is the establishment of the consistent size-dependent continuum mechanics theory. Recently, Hadjesfandiari and Dargush (2011) have resolved the troubles in the existing size-dependent continuum mechanics. This progress shows that the couple-stress tensor has a vectorial character and that the body couple is not distinguishable from the body force.

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In this theory, the stresses are fully determinate and the measure of deformation is the mean curvature tensor, which is the skew-symmetrical part of the macroscopic rotation gradient. This development can be considered the completion of the works of Mindlin and Tiersten (1962) and Koiter (1964). Furthermore, this size-dependent continuum mechanics must provide the fundamental base for developing different mechanical and electromechanical formulations that may govern the behavior of solid continua at the smallest scales. Here, the consistent size-dependent piezoelectric theory is developed, which shows that the size-dependent piezoelectric effect is related to the mean curvature tensor.

In the following section, we provide an overview of the electromechanical equations. This includes the equations for the kinematics, kinetics and quasi-electrostatics of size-dependent small deformation continuum mechanics. In Section 3, we consider the energy equation and its consequences based on the first law of thermodynamics for dielectric materials. In Section 4, the constitutive relations for linear elastic piezoelectric materials also are derived. Next, we develop two weak formulations in Section 5, which are used to establish conditions for uniqueness and to derive the reciprocal identity. Section 6 provides the general theory for isotropic linear material and the details for two dimensional cases are derived, including the closed form solution for polarization of a long cylinder in a uniform electric field. Finally, Section 7 contains a summary and some general conclusions.

2. Basic size-dependent electromechanical equations

Let us take the three dimensional coordinate system $x_1x_2x_3$ as the reference frame with unit base vectors $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$. Consider a piezoelectric elastic material continuum occupying a volume V bounded by a surface S. In size-dependent continuum theory, the interaction in the body is represented by true (polar) force-stress σ_{ij} and pseudo (axial) couple-stress μ_{ij} tensors. The force-traction vector $t_i^{(n)}$ and moment-traction vector $m_i^{(n)}$ at a point on surface element dS with unit normal vector n_i are given by

$$t_i^{(n)} = \sigma_{ji}n_j \tag{1}$$

$$m_i^{(n)} = \mu_{ji}n_j \tag{2}$$

The force-stress tensor is generally non-symmetric and can be decomposed as

$$\sigma_{ji} = \sigma_{(ji)} + \sigma_{[ji]} \tag{3}$$

where $\sigma_{(ji)}$ and $\sigma_{[ji]}$ are the symmetric and skew-symmetric parts, respectively. Hadjesfandiari and Dargush (2011) have shown that the axial couple-stress tensor is skew-symmetrical

$$\mu_{ji} = -\mu_{ij} \tag{4}$$

This means the moment-traction $m_i^{(n)}$ given by (2) is tangent to the surface. As a result, the couple-stress tensor μ_{ij} creates only bending moment-traction on any arbitrary surface in matter.

We can define the true (polar) couple-stress vector μ_i dual to the tensor μ_{ij} as

$$\mu_i = \frac{1}{2}\varepsilon_{ijk}\mu_{kj} \tag{5}$$

where ε_{ijk} is the permutation tensor or Levi–Civita symbol. This relation can also be written in the form

$$\varepsilon_{ijk}\mu_k = \mu_{ji} \tag{6}$$

Consequently, the surface moment-traction vector $m_i^{(n)}$reduces to

$$m_i^{(n)} = \mu_{ji}n_j = \varepsilon_{ijk}n_j\mu_k \tag{7}$$

which is obviously tangent to the surface.

To formulate the fundamental equations, we consider an arbitrary part of this electromechanical body occupying a volume V_a enclosed by boundary surface S_a. In infinitesimal deformation theory, the displacement vector field $\mathbf{u}(\mathbf{x}, t)$ is so small that the velocity and acceleration fields can be approximated by $\dot{\mathbf{u}}$ and $\ddot{\mathbf{u}}$, respectively. As a result, the linear and angular equations of motion for this part of the body are written as

$$\int_{S_a} t_i^{(n)}dS + \int_{V_a} F_i dV = \int_{V_a} \rho\ddot{u}_i dV \tag{8}$$

$$\int_{S_a} \left[\varepsilon_{ijk}x_j t_k^{(n)} + m_i^{(n)}\right]dS + \int_{V_a} \varepsilon_{ijk}x_j F_k dV = \int_{V_a} \varepsilon_{ijk}x_j\rho\ddot{u}_k dV \tag{9}$$

where F_i is the body force per unit volume of the body, and ρ is the mass density. Hadjesfandiari and Dargush (2011) have shown that the body couple density is not distinguishable from body force in size-dependent couple stress continuum mechanics and its effect is simply equivalent to a system of body force and surface traction.

By using the relations (1) and (2) for tractions in the equations of motion (8) and (9), along with the divergence theorem, and noticing the arbitrariness of volume, we finally obtain the differential form of the equations of motion as

$$\sigma_{ji,j} + F_i = \rho\ddot{u}_i \tag{10}$$

$$\mu_{ji,j} + \varepsilon_{ijk}\sigma_{jk} = 0 \tag{11}$$

Since the couple-stress tensor μ_{ji} is skew-symmetric, the angular equilibrium Eq. (11) gives the skew-symmetric part of the force-stress tensor as

$$\sigma_{[ji]} = -\frac{1}{2}\varepsilon_{ipq}\mu_{qp,j} = -\mu_{[i,j]} \tag{12}$$

Therefore, for the total force-stress tensor we have

$$\sigma_{ji} = \sigma_{(ji)} + \sigma_{[ji]} = \sigma_{(ji)} - \mu_{[i,j]} \tag{13}$$

As a result the linear equation of motion reduces to

$$[\sigma_{(ji)} - \mu_{[i,j]}]_{,j} + F_i = \rho\ddot{u}_i \tag{14}$$

It is seen that the sole duty of the angular equilibrium Eq. (11) is to produce the skew-symmetric part of the force-stress tensor.

In infinitesimal deformation theory, we may assume

$$\left|\frac{\partial u_i}{\partial x_j}\right| \ll 1, \quad \left|\frac{\partial^2 u_i}{\partial x_j \partial x_k}\right| \ll \frac{1}{l_S} \tag{15}$$

where l_S is the smallest characteristic length in the body. Therefore, the infinitesimal strain and rotation tensors are defined as

$$e_{ij} = u_{(i,j)} = \frac{1}{2}(u_{i,j} + u_{j,i}) \tag{16}$$

$$\omega_{ij} = u_{[i,j]} = \frac{1}{2}(u_{i,j} - u_{j,i}) \tag{17}$$

respectively. Since the true (polar) tensor ω_{ij} is skew-symmetrical, one can introduce it corresponding dual axial (pseudo) rotation vector as

$$\omega_i = \frac{1}{2}\varepsilon_{ijk}\omega_{kj} \tag{18}$$

The infinitesimal pseudo (axial) mean curvature tensor is also defined as

$$\kappa_{ij} = \omega_{[i,j]} = \frac{1}{2}(\omega_{i,j} - \omega_{j,i}) \tag{19}$$

Since this tensor is also skew-symmetrical, its corresponding dual polar (true) mean curvature vector is