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Size-dependent piezoelectricity: A 2D finite element formulation for electric field-mean curvature coupling in dielectrics

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ABSTRACT

The classical theory of piezoelectricity defines linear size-independent electromechanical response in non-centrosymmetric dielectrics that involves coupling between the electric field and the mechanical strains. However, with the continuing push to develop novel micro- and nano-scale materials, structures and devices, there is a need to refine and explore size-dependent electro-mechanical coupling phenomena, which have been observed in experiments on centrosymmetric dielectrics. Here a finite element variational formulation is developed based upon a recent consistent size-dependent theory that incorporates the interactions between the electric field and the mechanical mean curvatures in dielectrics, including those with centrosymmetric structure. The underlying formulation is theoretically consistent in several important aspects. In particular, the electric field equations are consistent with Maxwell's equations, while the mechanical field equations are based upon the recent consistent couple stress theory, involving skew-symmetric mean curvature and couple stress tensors. This, in turn, permits the development of a fully-consistent finite element method for the solution of size-dependent piezoelectric boundary value problems. In this paper, an overview of size-dependent piezoelectricity is first provided, followed by the development of the variational formulation and finite element representation specialized for the planar response of centrosymmetric cubic and isotropic materials. The new formulation is then applied to several illustrative examples to bring out important characteristics predicted by this consistent size-dependent piezoelectric theory.

1. Introduction

Over the last half-century, piezoelectric phenomena have had a profound impact on the development of many technologies. More recently, however, there is a push to develop technology on increasingly minute length scales, where it has been discovered that classical piezoelectric theory is not sufficient for describing all of the observed linear electromechanical coupling behavior. For modeling of small-scale electromechanical phenomena, a size-dependent piezoelectric theory, in some forms known as flexoelectricity, is necessary. These proposed theories are higher order continuum theories that include coupling between a higher order measure of deformation, such as strain-gradient or curvature, and the electric polarization field. Interestingly, it is shown both experimentally and theoretically that these size-dependent piezoelectric effects can occur in classically non-piezoelectric materials and, in particular, centrosymmetric cubic and isotropic materials.

Classical piezoelectricity describes the linear electromechanical coupling between strain or stress and the polarization within an anisotropic dielectric body. The groundbreaking experimental work of the Curie brothers established the foundation for piezoelectricity (Curie and Curie, 1880), which was subsequently placed on a firm theoretical base by Voigt (1910). The well-known monograph by Cady (1964) provides a comprehensive review of developments through the middle of the twentieth century. Since then countless technologies have taken advantage of piezoelectric phenomenon, from high-tech instrumentation to everyday commercial products.

Size-dependent piezoelectric effects were first discussed in Kogan (1964), Meyer (1969) and Tagantsev (1986) and were eventually coined “flexoelectric” effects. More recently size-dependent piezoelectric effects and electromechanical coupling effects in centrosymmetric bodies have been studied by numerous researchers (e.g., Mishima et al., 1997; Shvartsman et al., 2002; Buhlmann et al., 2002; Cross, 2006; Maranganti et al., 2006;

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Harden et al., 2006; Zhu et al., 2006; Sharma et al., 2007; Majdoub et al., 2008; Maranganti and Sharma, 2009; Resta, 2010; Baskaran et al., 2011; Catalan et al., 2011). With the increasing development of micro- and nano-scale technology, there is a need to model this size-dependent piezoelectric behavior, which can have useful effects for small characteristic geometries and cannot be captured using classical piezoelectric theory. This size-dependent behavior can be incorporated by considering that besides strain, the polarization in a dielectric body may be coupled to higher order measures of deformation as well. It is logical when formulating a size-dependent piezoelectric theory to consider a size-dependent elasticity theory and then introduce electromechanical coupling via thermodynamic considerations. Wang et al. (2004) consider the gradient of rotation as the higher order measure of deformation, which then is coupled to the polarization. Others have considered strain gradients and various forms of curvature to be coupled to the electric polarization (Tagantsev, 1986; Sharma et al., 2007; Eliseev et al., 2009). The previous theories suffer either from various incompatibility with the underlying Maxwell equations of electromagnetics (Hadjesfandiari, 2014) or with inherent indeterminacies due to the dependence on original couple-stress elasticity theories, as first developed by Toupin (1962), Mindlin and Tiersten (1962) and Koiter (1964).

Recently, the consistent couple-stress theory was developed, which remedied the issues that prior size-dependent elasticity theories had (Hadjesfandiari and Dargush, 2011, 2013). In this new theory, the mean curvature tensor is shown to be the correct higher order measure of deformation, while the skew-symmetric nature of the couple-stress tensor is revealed, making the theory fully determinate. More recently, in Hadjesfandiari (2013), a new consistent size-dependent piezoelectric theory is advanced by using the discoveries in Hadjesfandiari and Dargush (2011, 2013) regarding size-dependent elasticity. This new theory has coupling between the skew-symmetric mean curvature tensor and the polarization field, which allows for piezoelectric behavior even in centrosymmetric materials. Couple-stress effects are also inherently present in this theory (Hadjesfandiari, 2013).

In order for technology to take full advantage of piezoelectric phenomena, numerical methods for accurate modeling must be developed. Similar to most continuum theories, the only available analytical solutions for piezoelectric problems are based on very simple geometry and boundary conditions. To date, many finite element based formulations have been developed for modeling classical piezoelectricity. Benjeddou (2000) gives an excellent review of the advances in finite element approaches to modeling piezoelectric structural elements. Other notable works on finite element formulations for classical piezoelectricity include those of Allik and Hughes (1970) for applications to vibration, Hwang et al. (1993) for modeling of sensors and actuators, and Gaudenzi and Bathe (1995) for general continua analysis.

Despite the many efforts to advance numerical methods used to model and simulate classical piezoelectricity, very little work has been done in developing numerical methods to model size-dependent piezoelectric effects. Consequently, in this paper, we develop a mixed finite element (FE) formulation that can be applied to solve planar size-dependent piezoelectric problems. Because much work has already been done to develop finite element formulations for classical piezoelectric effects that can only exist in non-centrosymmetric anisotropic materials, we instead restrict ourselves to centrosymmetric materials. Most interestingly, higher order size-dependent piezoelectric effects can still be present for such materials, which in turn suggest many potential new applications at the micro- and nano-scale.

The formulation presented here is based on the consistent size-dependent piezoelectric theory of Hadjesfandiari (2013), while the finite element formulation can be considered an extension of the consistent couple-stress variational finite element approach developed by the present authors (Darrall et al., 2014). This new size-dependent piezoelectric FE formulation is based on the variational problem that is derived from considering the stationarity of a total electromechanical enthalpy functional. The electric field is coupled to the mean curvature within the electromechanical enthalpy, which allows for size-dependent piezoelectric effects. By considering the rotation to be an additional field variable and then enforcing rotation-displacement compatibility via Lagrange multipliers, the coupled size-dependent piezoelectricity problem is reduced to a C^0 variational problem. This type of formulation is made more attractive by the fact that these Lagrange multipliers are shown in Darrall et al. (2014) to be equal to the skew-symmetric portion of the stress tensor, which otherwise would be difficult to obtain in an efficient and accurate manner.

Throughout this paper, standard tensor index notation will be used where subscripts i, j, k, and l will range from 1 to 3 representing Cartesian coordinates x, y, and z. Repeating of indices implies summing over all values for that index. Additionally, ε_{ijk} is the Levi-Civita alternating symbol and δ_{ij} is the Kronecker delta. In Section 3, vector notation is used for convenience, where bold face characters will be used to represent vectors and matrices.

The remainder of the paper is organized as follows. Section 2 provides an overview of size-dependent piezoelectric theory for centrosymmetric materials and introduces the mixed variational principle upon which the finite element formulation is based. In Section 3, the corresponding finite element formulation is developed in detail. Then, in Section 4, we employ this new FE formulation to analyze four problems. First, the formulation is validated by comparing to the analytical solution of a long cylinder in a uniform electric field. The second problem analyzed is a cantilever subject to constant transverse electric field, which has significance to sensors and actuators. Results are compared to the beam model developed in Li et al. (2014). This same problem setting is then carried out for a cantilever consisting of Barium Titanate in the following subsection. These three problems all involve the converse size-dependent piezoelectric effect, in which an electric field induces a mechanical response. The final problem illustrates the direct size-dependent piezoelectric effect in isotropic media, having an electric field induced by an applied mechanical load. Finally, a number of conclusions are presented in Section 5.

2. Linear size-dependent piezoelectricity in a centrosymmetric material

In this section, a brief overview of the important concepts and relations of consistent size-dependent piezoelectricity theory is provided, based entirely on the work of Hadjesfandiari (2013). Particular attention is given to relations pertinent to the development of the finite element formulation presented in the next section. For a more detailed discussion on consistent size-dependent piezoelectricity, the reader is referred to Hadjesfandiari (2013).

At its simplest, linear size-dependent piezoelectricity can be described as the linear thermodynamic coupling between size-dependent elasticity and the electric polarization of a material. The theory presented here is based on the consistent skew-symmetric couple-stress theory (Hadjesfandiari and Dargush, 2011, 2013), which sets it apart from other size-dependent piezoelectricity and flexoelectricity theories. Furthermore, unlike the commonly accepted flexoelectric theory, the present formulation is consistent with Maxwell's equations of electromagnetism, which would seem to be a most important requirement. Details on the comparison can be found in Hadjesfandiari (2014). Because the present work is on size-dependent piezoelectricity as defined by