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Topology optimization of piezoelectric nanostructures

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ABSTRACT

We present an extended finite element formulation for piezoelectric nanobeams and nanoplates that is coupled with topology optimization to study the energy harvesting potential of piezoelectric nanostructures. The finite element model for the nanoplates is based on the Kirchoff plate model, with a linear through the thickness distribution of electric potential. Based on the topology optimization, the largest enhancements in energy harvesting are found for closed circuit boundary conditions, though significant gains are also found for open circuit boundary conditions. Most interestingly, our results demonstrate the competition between surface elasticity, which reduces the energy conversion efficiency, and surface piezoelectricity, which enhances the energy conversion efficiency, in governing the energy harvesting potential of piezoelectric nanostructures.

1. Introduction

Piezoelectric energy harvesters have garnered significant attention because of their ability to convert ambient mechanical energy into electrical energy (Priya, 2009, 2007). These energy harvesters have been utilized in a wide range of applications, where a review of vibration based energy harvesters is presented in Sodano et al. (2004).

Because of their wide usage, approaches to design piezoelectric energy harvesters with higher energy conversion efficiency have also been developed. One such approach is using computational topology optimization, where the geometry of the energy harvesters can be tuned to maximize the energy conversion efficiency. Examples of using topology optimization to design superior piezoelectric energy harvesters abound, including maximizing electromechanical conversion for a certain vibration mode (Silva and Kikuchi, 2007), designing a layout comprising the energy harvester as well as the electrical circuit (Rupp et al., 2009), and maximizing the energy conversion factor in cantilever plate energy harvesters subject to static loads (Zheng et al., 2009). There have also been works performing topology optimization of energy harvesters using different design variables, for example the densities that define the presence of piezoelectric material in each finite element

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(Nakasone and Silva, 2009), or the geometry of elastic substructure (Wein et al., 2013). In Chen et al. (2010), an approach for designing the optimal configuration of a cantilever and a cylindrical piezoelectric energy harvesters with single and multiple materials was presented. A procedure for converting an inverse problem of detecting flaws in piezoelectric structures into an iterative optimization problem was given in Nanthakumar et al. (2013, 2014, 2016).

However, most piezoelectric energy harvesters have been developed using bulk materials. The exciting possibility of using nanoscale piezoelectric energy harvesters emerged in 2006 with the discovery of piezoelectricity from ZnO nanowires by Wang and Song (2006). Many researchers have since extended the original seminal work, including the development of self-powered nano generators that can provide gate voltage to effectively control charge transport (Wang and Song, 2006), lateral and vertical integration of ZnO nanowires into arrays that are capable of producing sufficient power to operate real devices (Xu et al., 2010), and the experimental determination that the piezoelectric coefficient d_{33} of ZnO nanobelt is much larger compared to bulk ZnO through measurements made using piezoresponse force microscope (Zhao et al., 2004). A recent review on the electromechanical properties and performance of ZnO, and other piezoelectric nanostructures, was performed by Espinosa et al. (2012).

Along with experimental work, there have been some recent theoretical studies into the piezoelectric properties of nanostructures and nanowires. Dai et al. (2011) highlighted the concept of surface piezoelectricity using a combination of theory and atomistic calculations, and then analyzed the (0001) surfaces of ZnO. Other works have also found that ZnO nanostructures exhibit different piezoelectric properties as compared to bulk ZnO (Mitrushchenkov et al., 2009; Momeni et al., 2012a), while surface effects on the piezoelectricity of ZnO nanowires were studied by Dai and Park (2013). Using quantum mechanical calculations, Agrawal and Espinosa (2011) found substantial increases in the piezoelectric properties of ZnO and GaN nanowires with decreasing size, while an increase of piezoelectric coefficient to 2.322 C/m^2 compared to a bulk value of 1.4 C/m^2 when the nanobelt thickness decreases to 0.8 nm was obtained using a molecular dynamics model by Momeni et al. (2012b).

Other researchers have developed analytic models for surface elasticity and surface piezoelectricity. For surface elasticity, the seminal work was that of Gurtin, Murdoch and co-workers (Gurtin and Murdoch, 1975; Gurtin et al., 1998), who were the first to establish a surface or interface elasticity model to capture surface stress and elastic effects. The elastic properties of nanostructures with surface and interface effects using the extended finite element method (XFEM) were proposed by Yvonnet et al. (2008), and later extended by Farsad et al. (2010) to study the mechanical behavior of homogeneous and composite nanobeams. For surface piezoelectricity, various analytic models have been developed, including an explicit formula for the electromechanical coupling coefficient considering surface effects (Yan and Jiang, 2011a) for piezoelectric nanowires, an Euler–Bernoulli beam theory for the vibrational and buckling behavior of piezoelectric nanobeams (Yan and Jiang, 2011b), and the electroelastic response of thin piezoelectric places considering surface effects using Kirchoff plate theory (Wang, 2012). It is also worth emphasizing that the electromechanical coupling, and nanoscale piezoelectricity, should also be impacted by surface elastic effects, as experiments have shown that ZnO nanowires with diameter smaller than about 100 nm exhibit a dramatic increase in elastic modulus as compared to bulk ZnO (Chen et al., 2006).

The objective of this work is to develop and apply topology optimization techniques to study how surface electromechanical effects impact the energy conversion efficiency of piezoelectric ZnO nanostructures. We accomplish this by discretizing the equations of surface piezoelectricity using the extended finite element method (XFEM), and using this numerical formulation to study energy harvesting from piezoelectric nanowires, nanoplates, and piezoelectric layers in energy harvesters accounting for both surface elastic and surface piezoelectric effects. Our results demonstrate the relative effects of both surface elasticity and piezoelectricity on the electromechanical energy conversion efficiency, while also elucidating the difference in performance of the nanoscale energy converters under both open and closed circuit boundary conditions.

2. Governing equations of surface piezoelectricity

We consider a piezoelectric domain $\mathbf{\Omega}$ with a material surface $\mathbf{\Gamma}$. Based on the continuum theory of surface piezoelectricity (Dai et al., 2011), the equilibrium equations are

$$\nabla\cdot\boldsymbol{\sigma} + \boldsymbol{b} = 0 \quad \text{in } \mathbf{\Omega} \tag{1}$$

$$\nabla\cdot\mathbf{D} - \boldsymbol{q} = 0 \quad \text{in } \mathbf{\Omega} \tag{2}$$

$$\nabla_{\boldsymbol{s}}\cdot\boldsymbol{\sigma}_S = 0 \quad \text{on } \mathbf{\Gamma} \tag{3}$$

$$\nabla_{\boldsymbol{s}}\cdot\boldsymbol{D}_S = 0 \quad \text{on } \mathbf{\Gamma} \tag{4}$$

where $\boldsymbol{\sigma}$ and $\mathbf{D}$ are mechanical stress and electric displacement, respectively, while $\boldsymbol{\sigma}_{\mathbf{s}}$ and $\mathbf{D}_{\mathbf{s}}$ are the surface stress and the surface electric displacement, respectively. In the above equation, $\nabla_{\boldsymbol{s}}\cdot\boldsymbol{\sigma}_{\boldsymbol{s}} = \nabla\boldsymbol{\sigma}: \boldsymbol{P}$ and $\nabla_{\boldsymbol{s}}\cdot\boldsymbol{D}_{\boldsymbol{s}} = \nabla\boldsymbol{D}: \boldsymbol{P}$ where : is the double tensor contraction and where $\boldsymbol{P}$ is a second order tensor defined as $\boldsymbol{P} = \boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{n}$.

The linear piezoelectric constitutive relations for the bulk and surface are