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Nanoscale flexoelectric energy harvesting

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ABSTRACT

One of the most tantalizing applications of piezoelectricity is to harvest energy from ambient mechanical vibrations for powering micro and nano devices. However, piezoelectricity is restricted only to certain materials and is severely compromised at high temperatures. In this article, we examine in detail, the possibility of using the phenomenon of *flexoelectricity* for energy harvesting. The flexoelectric effect is universally present in *all* dielectrics and exhibits a strong scaling with size. Using a simple beam-based paradigmatical design, we theoretically and computationally examine flexoelectric energy harvesting under harmonic mechanical excitation. We find that the output power density and conversion efficiency increase significantly when the beam thickness reduces from micro to nanoscale and flexoelectricity-based energy harvesting can be a viable alternative to piezoelectrics. Specifically, the conversion efficiency in flexoelectric transduction at sub-micron thickness levels is observed to increase by two orders of magnitude as the thickness is reduced by an order of magnitude. The flexoelectric energy harvester works even for a single layer beam with a symmetric cross section which is not possible in piezoelectric energy harvesting. Our results also pave the way for exploration of high temperature energy harvesting since unlike piezoelectricity, flexoelectricity persists well beyond the Curie temperatures of the high electromechanical coupling ferroelectrics that are often used.

1. Introduction

Harvesting ambient waste energy into usable energy has received increasing attention over the last few years (Hudak and Amatucci, 2008; Elvin and Erturk, 2013). Efficient conversion of the ubiquitous ambient mechanical vibrations to electric energy for the powering of micro and nano systems, without the use of batteries, is an intensely researched subject. In particular, piezoelectric materials, as transducers between mechanical and electrical stimuli, are usually considered to be the ideal choice for such energy harvesting due to their high power density and ease of application (Anton and Sodano, 2007; Cook-Chennault et al., 2008; Priya, 2007). The applications of piezoelectric energy harvesting range from shoe-mounted inserts (Kymissis et al., 1998; Shenck and Paradiso, 2001) to unmanned aerial vehicles (Anton et al., 2012). Micro and nano implementations of piezoelectric energy harvesting have also received growing attention in the last few years due to the developments in ferroelectric thin films for MEMS (Trolier-McKinstry and Muralt, 2004; Jeon, 2005; Muralt et al., 2009) and non-ferroelectric nano wires NEMS (Wang and Song, 2006; Xu et al., 2010).

Recently, a somewhat understudied electromechanical coupling, *flexoelectricity*, has attracted a fair amount of attention from both fundamental and applications points of view leading to intensive experimental (Cross, 2006; Ma and Cross, 2001, 2002, 2003, 2006; Catalan et al., 2004; Zubko et al., 2007; Fu et al., 2006, 2007) and theoretical work (Sharma et al., 2007; Majdoub et al., 2009a; Eliseev et al., 2009, 2011; Maranganti and Sharma, 2009; Majdoub et al., 2008a,b, 2009b,c; Sharma et al., 2010, 2012; Gharbi et al., 2011; Kalinin and Meunier, 2008; Dumitrica et al., 2002). Piezoelectricity is restricted to only certain crystal structures and refers to a linear coupling between the development of polarization due to the action of *uniform* deformation and vice versa. In contrast, flexoelectricity links strain gradients to polarization and, in principle, exists in *all* dielectrics. In other words, even in non-piezoelectric materials, strain gradients can lead to the development of polarization. This effect is generally small but symmetry allows for its universal presence—unlike piezoelectricity. The reader is referred to the following articles for a detailed review: Refs. Tagantsev (1986, 2009), Maranganti et al. (2006), Nguyen et al. (2013) and Eliseev et al. (2011). Since strain gradient scales with feature size, and high values are easily obtainable at

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small length scales, flexoelectricity is expected to be significant at the micro and nanoscale possibly outperforming piezoelectricity in several scenarios. It is worth while to point out that flexoelectricity appears to have several ramifications for biophysics as well. For example, electromechanical transduction related to mammalian hearing appear to be dictated by flexoelectricity of biological membranes (Brownell et al., 2001, 2003; Raphael et al., 2000).

A commonly encountered problem in piezoelectric devices is *electric fatigue*. It is found that the switching polarization decreases significantly in some piezoelectric materials after some switching cycles (Jiang et al., 1994). Although the mechanism for this fatigue is still not full understood, some possible causes includes: transition of internal structure into a more stable configuration (Quarrie, 1953), the appearance of microcracks (Carl, 1975; Salaneck, 1972), and structural inhomogeneity which reduce the domain wall mobility (Williams, 1965). Since flexoelectricity allows a broader range of choices for the material, we can carefully choose those materials with higher fatigue resistance.

In this paper, we propose a flexoelectric energy harvester which shares some similarities but is, in many ways, quite different from the piezoelectric counterparts. The flexoelectric energy harvester is simpler in structure, allows a broader range of materials choice and exhibits strong size-scaling making it ideal for some micro scale and possibly all nanoscale applications. In Section 2, we present the main formulation and derive the requisite governing equations. In Section 3, we solve the simplest possible energy harvesting problem assuming harmonic base excitation. Based on the solution, the performance of the flexoelectric energy harvester is analyzed in Section 4. In particular, the size effect is studied in detail.

2. Electroelastic system and mathematical formulation

The flexoelectric energy harvester configuration investigated in this work is shown in Fig. 1. The flexoelectric cantilever beam is coated by perfectly conductive electrodes on its top and bottom surfaces. We assume that the electrode layers are very thin so that their contribution to the vibration of the cantilever can be neglected while their presence can easily be incorporated by preserving the centrosymmetry. The coordinate system and the resulting position coordinates x_1, x_2, x_3 are shown in Fig. 1. The longitudinal axis is denoted by x_1. The cantilever beam is mounted to a base moving in the x_3 direction. The transverse base displacement is denoted by $w_b(t)$. Due to the movement of the base, the cantilever beam undergoes bending vibrations. Dynamic strain gradient associated with vibration results in an alternating potential difference across the electrodes. The electrodes are connected to a resistive load (R) to quantify the electrical power output. Although the internal resistance of the dielectric beam is not taken into account, it can easily by considered as a resistor connected in parallel to the load resistance.

2.1. Variational principle for flexoelectricity

There are several approaches for formulating the electromechanical coupling in deformable materials. A particularly elegant

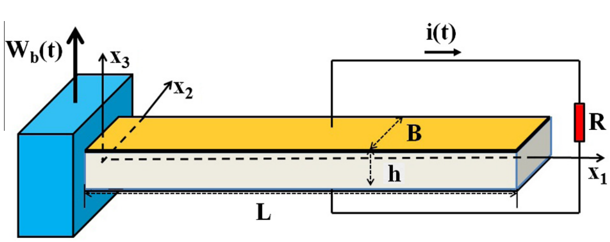

Fig. 1. A centrosymmetric flexoelectric energy harvester under base excitation.

exposition has been recently presented by Liu (2014). Based on Liu's work, Deng et al. (2014) studied the flexoelectricity in softmaterials. Other insightful works and alternative ways of formulating electrostatics of deformable bodies may also be referred to Dorfmann and Ogden (2005), McMeeking and Landis (2005), Suo et al. (2008), Steigmann (2009), Eringen and Maugin (1990) and Toupin (1956). Since the majority of the literature on linear active materials (such as piezoelectric dielectrics) follows Mindlin's approach (Mindlin, 1961, 1968; Tiersten, 1967), we have followed likewise.

Neglecting fringe fields, the variational principle for flexoelectric body can be written in the following form:

$$\delta\int_{t_1}^{t_2}dt\int_V\left[\frac{1}{2}\rho|\dot{\mathbf{u}}^m|^2-\left(W^L-\frac{1}{2}\epsilon_0|\nabla\phi|^2+\mathbf{P}\cdot\nabla\phi\right)\right]dV+\int_{t_1}^{t_2}dt\int_V\left(\mathbf{q}\cdot\delta\mathbf{u}^m+\mathbf{E}^0\cdot\delta\mathbf{P}\right)dV+\int_{t_1}^{t_2}dt\int_{\partial V}\tilde{D}\delta\phi dA=0 \tag{1}$$

where $\mathbf{u}^m$ and ϕ are the absolute displacement and potential field in the beam, $\mathbf{P}$ is the polarization density, W^L is the internal energy density, $\mathbf{q}$ and $\mathbf{E}^0$ correspond to the external body force and the external electric field, respectively. Because of the conductive electrodes coated on the surface, a boundary integration term is added here. This last term corresponds to the virtual work done by moving charges on to or out of the electrodes as a product of the variation of potential ϕ and the average electric displacement $\tilde{D}$. Note that the bulk electric displacement is related to the polarization by $-\epsilon_0\nabla\phi+\mathbf{P}$.

At the outset we assume a linearized setting. Then the internal energy density W^L can be written as (Sahin and Dost, 1988; Sharma et al., 2007)

$$W^L=\frac{1}{2}\mathbf{P}\cdot\mathbf{aP}+\frac{1}{2}\mathbf{S}\cdot\mathbf{cS}+\mathbf{P}\cdot\mathbf{dS}+\mathbf{P}\cdot\mathbf{f}\nabla\nabla\mathbf{u}+\frac{1}{2}\nabla\nabla\mathbf{u}\cdot\mathbf{g}\nabla\nabla\mathbf{u} \tag{2}$$

where $\mathbf{u}$ is the displacement field relative to the moving base $\mathbf{u}=\{u_1^m,u_2^m,u_3^m-w_b(t)\}^T$, $\mathbf{S}=\frac{1}{2}(\nabla\mathbf{u}+(\nabla\mathbf{u})^T)$ is the infinitesimal strain tensor, and $\nabla\nabla\mathbf{u}$ is the strain gradient tensor. The coefficients $\mathbf{a},\mathbf{c},\mathbf{d},\mathbf{f}$, and $\mathbf{g}$ are material properties, i.e., $\mathbf{a}$ is the reciprocal dielectric susceptibility which relates to relative permittivity ϵ_r and the vacuum permittivity ϵ_0 by $\mathbf{a}=\frac{1}{(\epsilon_r-1)\epsilon_0}$, $\mathbf{c}$ corresponds to elastic modulus, $\mathbf{d}$ and $\mathbf{f}$ are the piezoelectric and flexoelectric constants, respectively. The parameter $\mathbf{g}$ is nonzero only if the strain gradient is considered. $\mathbf{g}$ relates strain gradient $\nabla\nabla\mathbf{u}$ to its energy conjugate, high order stress tensor (Majdoub et al., 2008a).

The base movement $w_b(t)$ is the given Dirichlet boundary condition, so we have $\delta\mathbf{u}^m=\delta\mathbf{u}$. For independent $\mathbf{P},\mathbf{u}$, and ϕ, we have

$$\delta\int_{t_1}^{t_2}dt\int_V\left[W^L-\frac{1}{2}\epsilon_0|\nabla\phi|^2+\mathbf{P}\cdot\nabla\phi\right]dV=\int_{t_1}^{t_2}dt\int_V\left[\frac{\partial W^L}{\partial\mathbf{P}}\delta\mathbf{P}+\frac{\partial W^L}{\partial\mathbf{S}}\delta\mathbf{S}+\frac{\partial W^L}{\partial\nabla\nabla\mathbf{u}}\delta(\nabla\nabla\mathbf{u})-\epsilon_0\nabla\phi\delta(\nabla\phi)+\mathbf{P}\delta(\nabla\phi)+\nabla\phi\delta\mathbf{P}\right]dV \tag{3}$$

and

$$\delta\int_{t_1}^{t_2}dt\int_V\frac{1}{2}\rho|\dot{\mathbf{u}}^m|^2dV=-\int_{t_1}^{t_2}dt\int_V\rho\ddot{\mathbf{u}}^m\delta\mathbf{u}dV$$

Then, from Eq. (1), we have the Euler–Lagrange equations

$$\begin{aligned}&Div\left[\frac{\partial W^L}{\partial\mathbf{S}}-Div\left(\frac{\partial W^L}{\partial\nabla\nabla\mathbf{u}}\right)\right]+\mathbf{q}=\rho\ddot{\mathbf{u}}^m\\&\frac{\partial W^L}{\partial\mathbf{P}}+\nabla\phi=\mathbf{E}^0\\&Div(-\epsilon_0\nabla\phi+\mathbf{P})=0\end{aligned} \tag{4}$$

in the domain V and the corresponding boundary conditions