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Modeling of a nanoscale flexoelectric energy harvester with surface effects

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ABSTRACT

This work presents the modeling of a beam energy harvester scavenging energy from ambient vibration based on the phenomenon of flexoelectricity. By considering surface elasticity, residual surface stress, surface piezoelectricity and bulk flexoelectricity, a modified Euler-Bernoulli beam model for the energy harvester is developed. After deriving the requisite energy expressions, the extended Hamilton's principle and the assumed-modes method are employed to obtain the discrete electromechanical Euler-Lagrange's equations. Then, the expressions of the steady-state electromechanical responses are given for harmonic base excitation. Numerical simulations are conducted to show the output voltage and the output power of the flexoelectric energy harvesters with different materials and sizes. Particular emphasis is given to the surface effects on the performance of the energy harvesters. It is found that the surface effects are sensitive to the beam geometries and the surface material constants, and the effect of residual surface stress is more significant than that of the surface elasticity and the surface piezoelectricity. The axial deformation of the beam is also considered in the model to account for the electromechanical coupling due to piezoelectricity, and results indicate that piezoelectricity will diminish the output electrical quantities for the case investigated. This work could lead to the development of flexoelectric energy harvesters that can make the micro- and nanoscale sensor systems autonomous.

1. Introduction

With the miniaturization and integration of electronic components, developing miniature power packages and self-powering techniques will be the key challenge in a variety of applications, including wireless sensing, environmental monitoring, implantable medical devices, personal electronics and etc. Consequently, researchers are developing innovative nano-technologies to generate or store the electrical energy created from ambient environment for low-power nanodevices. In particular, nanostructured piezoelectric materials, which can directly generate electric charges when mechanically deformed, have attracted significant attention for building energy harvesters in the last decade. In 2006, Wang and Song [1] demonstrated the first piezoelectric nanogenerator for converting mechanical energy into electricity using ZnO nanowires. Subsequently, energy harvesters of various designs based on the piezoelectric effect have been demonstrated [2–5]. Besides, triboelectric nanogenerators have recently been successfully fabricated based on the electrostatic effect [6,7]. In principle, a technique that is capable of generating electric charges can be exploited to develop energy-harvesting devices. Therefore, a spontaneous electric polarization induced by a non-uniform strain field (or strain gradient), termed as flexoelectricity, is highly possible to achieve such a purpose.

The flexoelectric effect was discovered in the 1950s [8], but very limited attention was paid to it for a long period of time due to its expected weak effect. The revival of scientific interest in flexoelectricity started from the early 2000s. At that time, Ma and Cross [9–12] measured the flexoelectric coefficients of a series of materials such as relaxor and ferroelectric dielectrics, and found that the measured constants were remarkably larger than expected. Their experiments also confirmed the prediction made by Tagantsev [13] that the flexoelectric coefficient of a material is proportional to its dielectric constant. Since the strain gradient becomes more manifest with the decrease of the characteristic size of the structure, the strain-gradient associated flexoelectric effect is a size-dependent property and becomes significant at the nanoscale. Naturally, flexoelectricity gains more and more attention with the growing interest in nanoscience. Flexoelectricity has been found to play an important role in the physical properties of ferroelectric thin films and is responsible for some unusual electromechanical behaviors that emerged at submicron scales, such as asymmetry of polarization hysteresis curves [14], polarization switch [15] and polarization rotation [16]. In addition, the physical and mathematical formulations for dielectrics have been

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developed to account for the flexoelectric effect. As examples, Catalan et al. [17] presented a phenomenological model for ferroelectric thin films and considered the flexoelectricity by adding two extra terms to the conventional Landau-Ginzburg-Devonshire (LGD) free energy expression. Maranganti et al. [18] developed a general formulation for dielectrics including the flexoelectric effect based on the variational principle and provided Green's function solutions for the governing equations of an isotropic centrosymmetric continuum medium. Shen and Hu [19] established a more comprehensive framework for nanoscale dielectrics with the consideration of surface effects in addition to flexoelectricity. Later, extensive studies have been conducted to understand the influence of flexoelectric effect on the electromechanical coupling properties of various nanostructures [20–25]. The exploitation of flexoelectricity also leads to tantalizing applications. For example, the flexoelectric control of defect formation allows a nearly defect-free film with fully functional electronic properties [26]. Since flexoelectricity occurs in all 32 crystallographic point groups, unlike piezoelectricity which exists only in 20 noncentrosymmetric point groups, one interesting application of flexoelectricity is to create apparently piezoelectric materials without using piezoelectric materials [27]. Chandratre and Sharma [28] numerically validated such an idea, they considered a graphene nanoribbon impregnated with holes and found that the artificially structured material would exhibit piezoelectricity as long as certain symmetry rules of holes were followed. In a similar vein, Zelisko et al. [29] confirmed in their work that flexoelectricity and triangular defects cause graphene nitride to exhibit an apparent piezoelectricity. As piezoelectric nanomaterials have gained popularity for energy harvesting, not surprisingly, the potential for the use of flexoelectricity in energy harvesting has also been addressed by researchers. For instance, significant enhancement of the piezoelectric coefficient of a piezoelectric nanobeam/ribbon due to flexoelectric effect was reported [3,30], which is essential for energy harvesting applications. Deng et al. [31] have developed a theoretical continuum model for flexoelectric nanoscale energy harvesting. Very recently, Wang and Wang [32] presented an analytical model for nanoscale unimorph piezoelectric energy harvesters with the flexoelectric effect. Their results showed that the flexoelectric effect can play a major role in the energy harvesting of piezoelectric cantilever nanobeams. However, the flexoelectric energy harvesting is still a burgeoning concept and its fundamental principles governing the energy conversion need to be further understood.

On the other hand, surface effects are widely recognized to significantly affect the mechanical and physical properties of nanoscale structures. Based on Gurtin and Murdoch's [33] linear surface elasticity theory and its extended theories, a great number of studies have been conducted to examine the influence of surface effects on static and dynamic behaviors of elastic and piezoelectric nanomaterials [34–38]. As the size of an energy harvester reduced to nanoscale, it is natural to believe that surfaces effect will influence its energy-harvesting performance. Taking surface effects into consideration, Wang and Wang [39] studied the energy-harvesting performances of a piezoelectric circular nanomembrane under human blood pressure; Fan and Yang [40] examined a nano energy harvester under flexural vibration. However, the working mechanism of these energy harvesters are based on the effect of piezoelectricity, rather than flexoelectricity. In this work, a comprehensive continuum model of a nanoscale flexoelectric energy harvester under harmonic base excitation is developed. The surface effects including surface elasticity, residual surface stress and surface piezoelectricity as well as the effect of beam axial deformation are incorporated into the model. The performance of the proposed flexoelectric energy harvesters is revealed and discussed. The proposed energy harvester provides a solution for energy harvesting at the nanoscale. Since it is based on a simple structure that can be made of a wide range of materials, it is perhaps even better than piezoelectric nanogenerators under some extreme conditions and is thus ideal for mirco- and nanoscale applications.

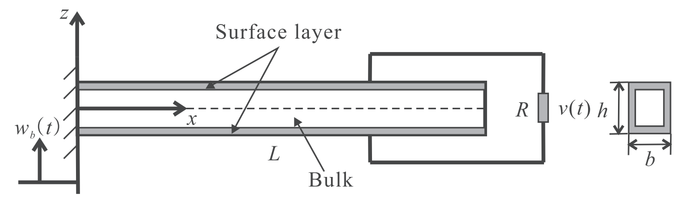

Fig. 1. Schematic of a flexoelectric beam energy harvester under base excitation and cross-sectional view of the cantilever beam.

2. Euler-Bernoulli model of a flexoelectric energy harvester with surface effects

Consider a flexoelectric beam energy harvester configuration shown in Fig. 1, L, b and h are the beam length, width and thickness, respectively. The configuration has a single flexoelectric bulk core made of piezoceramic and the circumferential surfaces are adhering to the bulk with negligible thickness. A Cartesian coordinate system (x, y, z) is used to describe the beam, where x-axis is along the beam longitudinal direction and z-axis is along the beam thickness direction, which is also the poling direction of the piezoelectric body. The beam is mounted to a base moving in the z direction with the transverse base displacement being denoted by $w_b(t)$. It is assumed that the conductive electrodes fully cover the upper and lower surfaces of the beam and are directly connected to a resistive load R. The voltage across the resistor R is $v(t)$, which can be regarded as the output voltage of the flexoelectric energy harvester.

Based on the Euler-Bernoulli beam model, the displacement fields at any point in the beam and time t can be defined as

$$u(x, z, t) = u^0(x, t) - z\frac{\partial w(x, t)}{\partial x}; \quad w(x, z, t) = w(x, t) \tag{1}$$

where $u^0(x, t)$ is the axial displacement along the centroidal axis of the beam and $w(x, t)$ is the transverse displacement relative to the moving base. Accordingly, the axial strain ε_x and the strain gradient $\varepsilon_{x,z}$ can be written as

$$\varepsilon_x = \frac{\partial u^0(x, t)}{\partial x} - z\frac{\partial^2 w(x, t)}{\partial x^2}; \quad \varepsilon_{x,z} = -\frac{\partial^2 w(x, t)}{\partial x^2} \tag{2}$$

It should be mentioned that the strain gradient $\varepsilon_{x,x}$ is small as compared to $\varepsilon_{x,z}$ for a thin beam and thus is not considered here [20]. The electric field in the beam is assumed to exist only in the z-direction and expressed as $E_z = -v(t)/h$, which also indicates that the gradient of the electric field in the piezoelectric beam is zero. Therefore, the expression for the bulk electric Gibbs free energy density function u_b of the beam including the strain gradient induced flexoelectricity can be written as

$$u_b = -\frac{1}{2}a_{33}E_z^2 + \frac{1}{2}c_{11}\varepsilon_x^2 - e_{31}E_z\varepsilon_x - f\varepsilon_{x,z}E_z + \frac{1}{2}g\varepsilon_{x,z}^2 \tag{3}$$

where c_{11}, e_{31} and a_{33} are the bulk elastic, piezoelectric and dielectric constants, respectively. f is the direct flexoelectric constant and g represents the purely non-local elastic effect.

Then the total bulk energy in the volume (V) of the structure is

$$U_b = \int_V u_b \mathrm{d}V = \frac{1}{2}b\int_0^L \left\{c_{11}h\left[\frac{\partial u^0(x, t)}{\partial x}\right]^2 + \left(\frac{c_{11}h^3}{12} + gh\right)\left[\frac{\partial^2 w(x, t)}{\partial x^2}\right]^2 + 2e_{31}v(t)\frac{\partial u^0(x, t)}{\partial x} - 2fv(t)\frac{\partial^2 w(x, t)}{\partial x^2} - a_{33}\frac{[v(t)]^2}{h}\right\}\mathrm{d}x \tag{4}$$

The surface energy U_s of the investigated beam with a surface area a can be expressed as [41]

$$U_s = \int_a \left[\frac{1}{2}(\sigma_0 + \sigma_x^s)\varepsilon_x^s\right]\mathrm{d}a \tag{5}$$

where σ_0 is the residual surface stress, ε_x^s is the axial surface strain, and σ_x^s is the axial surface stress and can be expressed by

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