Numerical Analysis of Piezoelectric Nanobeams with Flexoelectric Effect

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Abstract

Cutting edge composite materials now play an essential role in micro/nano-structural systems. Micro/ Nano particles and/or structural systems are embedded into a material matrix in order to enhance material properties, and make them a "smart material". A widely used type of smart material is piezoelectric materials, which have the property of piezoelectricity - an electromechanical effect that occurs in some micronano- structural materials. A further electromechanical effect called the flexoelectric effect is also induced due to the fact that strain gradient on the micro/nano scale provides an electrical polarization. In this work, the Finite Element Method (FEM) formulation for beam theories is used to investigate materials including both piezoelectric and flexoelectric effects. The variational form of 2D piezoelectric nanobeams with flexoelectric effect is also presented and solved using FEM. The results from beam theories and 2D planar beams will be compared with analytical solutions and other numerical techniques.

Keywords: Finite element Method, Piezoelectric Nanobeam, flexoelectric effect.

1. Introduction

With the advancement of electro-mechanic technology, the nano-structure devices have attracted many researchers' enthusiasm and size-dependent effects of materials have become one of the hottest topics.

Piezoelectricity, first discovered in 1880 by French physicists Jacques and Pierre Curie, is the electrical polarization in response to applied mechanical stress. In

2009, Maranganti and Sharma [1] gave a more explicit definition of piezoelectricity: Upon application of a uniform strain, internal sub-lattice shifts within the unit cell of a non-centrosymmetric dielectric crystal result in the appearance of a net dipole moment. It has also been observed that the piezoelectric effect is symmetric in the sense that charge separation occurs due to stress (the direct piezoelectric effect) and stress and strain are induced when an electric field is applied (inverse piezoelectric effect).

The flexoelectric effect is a further electromechanical effect in insulating materials in which gradients in the strain induce an electrical polarisation. The similarity between piezoelectricity and flexoelectricity is that both produce polarizations, however they differ in that piezoelectricity is a macroscopic effect while flexoelectricity is a microscopic one. Therefore, theories of strain-gradient elasticity are needed to predict the response of a micro/nano beam when the flexoelectric effect is involved. Toupin [4] put forward a variational principle for a linear piezoelectric material. The polarization can be also induced by a strain gradient, which is the well known "flexoelectric effect". The contributed polarization in response to macroscopic strain gradient can be written as

$$P_l = f_{ijkl} \frac{\partial \varepsilon_{ij}}{\partial x_k} \quad (1)$$

Where P_l denote the component of resultant polarization, f_{ijkl} is the flexoelectric coefficients, ε_{ij} is the component of the elastic strain and x_k is the direction of the gradient.

A lot of pioneering work investigating flexoelectric effect has been undertaken. Yan and Jiang [5] acquired the electromechanical coupling behavior of piezoelectric nanowires with Bernoulli-Euler Beam theory. Two years

after, they investigated the flexoelectric effect on the bending of piezoelectric nano-beams by different boundary conditions with different beams theories. In 2014, Liang et al. [6] incorporated the flexoelectric and surface effect into his Bernoulli-Euler beam model, and solved them analytically.

In this paper, the one dimensional beam theories will be used to simulate the beam's behavior along with piezoelectricity and flexoelectricity. The new 2D beam models for piezoelectric nanobeams with the flexoelectric effect will be expressed.

2. Formulation

The development of a continuum electromechanical coupling framework by Hu et al. [7] has resulted in a great deal of interest in nanobeam modelling including the flexoelectric effect. Taking the flexoelectric effect into account, the bulk electric Gibbs free energy has been proposed as a hybrid of the internal energy of elastic deformation and electrostatic field.

$$U_b = -\frac{1}{2}a_{ij}E_iE_j + \frac{1}{2}c_{ijkl}\varepsilon_{ij}\varepsilon_{kl} - d_{ijk}E_i\varepsilon_{jk} - f_{ijkl}E_i\eta_{jkl} \quad (2)$$

where a_{ij} , c_{ijkl} , d_{ijk} and f_{ijkl} denote second-order permittivity, four-order elastic, piezoelectric and flexoelectric tensors, respectively. The other terms are the strain tensor, ε_{ij} , the strain gradient tensor, η_{jkl} , and the electric field tensor, E_i . Here, the constitutive equations [6] are

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} - d_{kij}E_k \quad (3)$$

$$\tau_{jkl} = f_{ijkl}E_i \quad (4)$$

$$D_i = a_{ij}E_j + d_{ijk}\varepsilon_{jk} + f_{ijkl}\eta_{jkl} \quad (5)$$

where σ_{ij} is the classical stress tensor, D_i is the electrical displacement vector and τ_{jkl} is the high-order stress tensor. Substituting these into Eq. 2, the final form of the bulk electric Gibbs energy can be rewritten as

$$U_D = \frac{1}{2}\sigma_{ij}\varepsilon_{ij} + \frac{1}{2}\tau_{jkl}\eta_{jkl} - \frac{1}{2}D_kE_k \quad (6)$$

and these can be expressed in the variational form as:

$$\int_V \delta\varepsilon_{ij}\sigma_{ij}dV + \int_V \delta\eta_{jkl}\tau_{jkl}dV - \int_V \delta E_k D_k = 0 \quad (7)$$

Written with these variables, the variational form of Eq. 7 appears similar to that of the strain gradient elasticity theory of the strain gradient elasticity theory [8] with the addition of an electric term. Eq. 2 can be written as in variational form as [8]:

$$\begin{aligned} & \int_V \delta\varepsilon_{ij}C_{ijkl}\varepsilon_{kl}dV - \int_V \delta\varepsilon_{ij}d_{kij}E_kdV - \int_V \delta\eta_{jkl}f_{ijkl}E_idV \\ & - \int_V \delta E_k a_{ij}E_jdV - \int_V \delta E_k d_{ijk}\varepsilon_{jk}dV - \int_V \delta E_k f_{ijkl}\eta_{jkl}dV = 0. \end{aligned} \quad (8)$$

For 2D beam models in the x-z plane, the internal energy of elastic deformation can be written as [9]

$$U_b = \frac{1}{2}\sigma_1\varepsilon_1 + \frac{1}{2}\sigma_{13}\varepsilon_{13} + \frac{1}{2}\tau_{113}\eta_{113} - \frac{1}{2}\varepsilon_0E_3E_3 - \frac{1}{2}P_3E_3 \quad (9)$$

As shown through this section the variational form was derived from the Principal of the Principal of Virtual Work and these can be solved using well known simulation tools, such as Finite element methods.

3. Numerical Results

Piezoelectric nanobeams under different conditions are analysed with the variation of the aspect ratios ($L/h = 5, 10, 15, 20$). The deflection (w) of beams are observed and these will be compared with the validated results of the 1D piezoelectric nanobeam. In the comparisons, $Error_{(EB-TB)}$ and $Error_{(2D-TB)}$ are defined.

$$Error_{(EB-TB)} = \left| \frac{w^{EB} - w^{TB}}{w^{TB}} \right| \times 100\% \quad (8)$$

$$Error_{(2D-TB)} = \left| \frac{w^{2D} - w^{TB}}{w^{TB}} \right| \times 100\% \quad (9)$$

Where the subscripts and superscripts represent the beam theories used: Euler-Bernoulli beam (EB), Timoshenko beam

(TB) and 2D planar beam.

Table 1. Beam deflection (nm) with different boundary condition: clamp-clamped beam, simply-supported beam and cantilever beam when $L/h=5$.

Clamp-Clamped beam (CC)	$L/h = 5$		
	Classical	$V^n=0$	$V^n=1$
1D(EB)	0.02982	0.02312	0.02314
1D(TB)	0.04729	0.04060	0.04066
Error _(EB-TB)	36.94%	43.05%	43.08%
2D plane	0.04660	0.03873	0.03901
Error _(2D-TB)	1.46%	4.58%	4.06%
Simply-Supported beam (SS)	$L/h = 5$		
	Classical	$V^n=0$	$V^n=1$
1D(EB)	0.14909	0.11559	0.25716
1D(TB)	0.16655	0.13305	0.27488
Error _(EB-TB)	10.48%	13.12%	6.45%
2D plane	0.17211	0.13730	0.27950
Error _(2D-TB)	3.33%	3.19%	1.68%
Cantilever beam (CT)	$L/h = 5$		
	Classical	$V^n=0$	$V^n=1$
1D(EB)	1.4313	1.1096	0.5446
1D(TB)	1.5012	1.1796	0.6273
Error _(EB-TB)	4.66%	5.93%	13.19%
2D plane	1.4999	1.1744	0.6223
Error _(2D-TB)	0.09%	0.44%	0.8%

Table 1 shows the deflection of beam with the aspect ratio of 5. The "Classical" column represents the beam without the size-dependent effect.

Table 2. Beam deflection (nm) with different boundary condition: clamp-clamped beam, simply-supported beam and cantilever beam when $L/h=10$.

Clamp-Clamped beam (CC)	$L/h = 10$		
	Classical	$V^n=0$	$V^n=1$
1D(EB)	0.02982	0.02312	0.02314
1D(TB)	0.03418	0.02748	0.02751
Error _(EB-TB)	12.75%	15.87%	15.88%
2D plane	0.03411	0.02714	0.02727
Error _(2D-TB)	0.21%	1.25%	0.88%
Simply-Supported beam (SS)	$L/h = 10$		
	Classical	$V^n=0$	$V^n=1$
1D(EB)	0.14909	0.11559	0.25716
1D(TB)	0.15344	0.11994	0.26157

Error _(EB-TB)	2.83%	3.62%	1.69%
2D plane	0.15412	0.12035	0.26208
Error _(2D-TB)	0.44%	0.34%	0.19%
Cantilever beam (CT)	$L/h = 10$		
	Classical	$V^n=0$	$V^n=1$
1D(EB)	1.4313	1.1096	0.5446
1D(TB)	1.4488	1.1271	0.5740
Error _(EB-TB)	1.21%	1.55%	5.13%
2D plane	1.4486	1.1262	0.5733
Error _(2D-TB)	0.01%	0.08%	0.13%

Table 2 shows the deflection of beam with the aspect ratio of 10. It is noted that the displacements calculated from EB theory are unchanged though the aspect ratio under the same loads, whereas the deflections calculated by TB theory changed. This may be due to the fact that TB theory considers the effect of shear deformation in beams, resulting in the observation of a big difference between the results from 1D(EB) and 1D(TB).

In order to illustrate the results more evidently, the data from Table 1 and 2 is presented in Figure 1, where the horizontal axis represents the aspect ratio ($L=h$) and the vertical axis represents the percentage error.

Figure 1. Errors for clamped-ends beams VS aspect ratio

After looking into the tables deeply, the contribution of electrical load is relatively small for CC beams, comparing with the SS beams and CT beams. This shows the analysis of a piezoelectric nanobeam indicating the flexoelectric effect.

4. Conclusions

The results show that the flexoelectric effect plays a more essential role in the behavior of materials at micro/nano scale than the piezoelectric effect. Under a purely mechanical load ($V^n=0$), flexoelectricity acted to stiffen the beams, as can

be seen from the reduced deflection. Under an external electrical load ($V_n=1$), with cantilever beams subjected to a positive voltage, flexoelectricity plays an essential role in preventing bending, greatly reducing the beam displacement.

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