Influence of Surface Effects and Flexoelectricity on Vibration of Piezoelectric Nanobeams

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Abstract Nanostructured piezoelectric materials hold a promise for the development of novel nanodevices in nanoelectromechanical systems (NEMS) due to their efficient electromechanical coupling. To fulfill their potential applications, it is essential to quantitatively predict their fundamental physical and mechanical properties. In this work, the unique size-dependent properties of piezoelectric nanomaterials, which are believed to attribute to surface effects and flexoelectricity, are investigated through a modified Euler beam model. The surface effects are accounted in a modified beam theory through the surface piezoelectricity model and the generalized Young-Laplace equations, while the flexoelectricity is considered by using the higher-order theory of piezoelectricity. Simulation results on the vibration analysis of piezoelectric nanobeams reveal that the influence of surface effects and flexoelectricity varies with beam thickness and aspect ratio, in particular, such influence becomes more pronounced with the decrease of beam thickness. Vibration analysis also identifies possible frequency tuning of piezoelectric nanobeams by electrical load. In addition, the effect of axial boundary constraints in modeling has been studied, which provides a clear interpretation on the relaxation phenomenon of nanobeams under certain boundary constraints. This study is expected to provide a quantitative understanding on the fundamental physics of piezoelectric materials, thus leading to a better design for piezoelectric nanobeam-based devices.

Keywords Surface effects, Flexoelectricity, Size-dependent properties, Piezoelectric nanobeam

1. Introduction

One-dimensional piezoelectric nanostructures, such as piezoelectric nanowires, nanobelts and nanorods have been extensively used in nanoelectromechanical systems (NEMS) as nanosensors [1], nanoresonators [2] and nanogenerators [3, 4]. The superior performances exhibited by these devices can be attributed to the novel electromechanical coupling properties of piezoelectric materials at nanoscale. Therefore, to reveal the underlying physical mechanisms of piezoelectric nanomaterials and to achieve the unprecedented improvements of these nanosized devices, it is essential to conduct a quantitative study on the physical and mechanical properties of nanostructured piezoelectric materials.

"Small is different", it is expected that the physical properties of piezoelectric nanomaterials differ from their bulk counterparts. Efforts have been devoted to investigating the physical properties of piezoelectric nanostructures. For example, it was experimentally observed that the elastic and fracture properties of piezoelectric nanowires demonstrated a size-dependent behavior unlike the bulk piezoelectric wires [5, 6]. The size-dependent mechanical properties of piezoelectric nanomaterials have also been confirmed by conducting atomistic modeling and simulations [7]. Based on a molecular dynamics study, the size effects were found to have a prominent influence on the polarization distribution, piezoelectric coefficient and hysteresis behaviors of BaTiO₃ nanowires [8]. All the aforementioned studies indicated the size effects played a significant role in predicting the mechanical and physical properties of piezoelectric nanostructures. In parallel to experimental work and atomistic studies, continuum mechanics modeling, as an alternative and efficient tool, has been naturally resorted to investigate the mechanical properties of nanostructured materials. However, classical continuum approaches, which ignore the variation of interatomic quantities, fail to capture the size effects of materials at nanoscale. Therefore, non-classical continuum models with the consideration of size effects are necessary to conduct the mechanical and physical analysis of nanoscale structures.

Due to the large surface area to volume ratio of typical nanostructures, surface effects are believed to attribute to the size-dependent properties of these structures. By taking into account of surface effects, Gurtin and Murdoch proposed a surface elasticity model for elastic materials [9], in which a surface is modeled as a thin layer with negligible thickness adhered to the bulk without slipping, and the constitutive and equilibrium equations for the surface layer are different from those in the bulk of the solid. Using this model, the size-dependent properties of elastic nanomaterials have been successfully predicted [10-12]. However, the surface elasticity model is not sufficient to investigate the mechanical behaviors of piezoelectric nanostructures with electromechanical coupling properties. In order to solve this problem, modified continuum model with electric field dependent surface effects has been developed for piezoelectric nanostructures [13]. In this surface piezoelectricity model, the surface stresses depend on surface piezoelectricity in addition to surface elasticity and residual surface stress incorporated in the surface elasticity theory. Based on this novel surface piezoelectricity model, the static and dynamic behaviors of various piezoelectric nanostructures have been investigated [13-16]. Simulation results indicated that the surface effects had a significant influence on the static bending, vibration and mechanical buckling properties of these piezoelectric nanostructures.

In literature, flexoelectricity was also believed to be responsible for the size-dependent properties of piezoelectric nanomaterials, which refers to a spontaneous polarization of dielectric materials due to a strain gradient or a non-uniform strain field. Maranganti *et al.* proposed a theoretical framework for dielectrics with the consideration of flexoelectricity, elucidating the mechanism for size-dependent electromechanical coupling due to strain or polarization gradients [17]. The strong size-dependent enhancement of the effective piezoelectric coefficients of piezoelectric nanomaterials was demonstrated by Majdoub *et al.* [18] with the incorporation of flexoelectricity into piezoelectricity theory. Eliseev *et al.* investigated the renomalization in properties of nanoferroics due to spontaneous flexoelectric effect [19]. Recently, Liu *et al.* studied the effect of flexoelectricity on electrostatic potential in a piezoelectric nanowire [20]. These existing studies indicated the necessity of considering flexoelectric effect in characterizing the properties of nanostructured piezoelectric materials.

The objective of this work is to conduct the vibration analysis of a piezoelectric nanobeam with the consideration of surface effects and flexoelectricity. The surface effects are accounted in a modified beam theory through the surface piezoelectricity model and the generalized Young-Laplace equations. It should be mentioned that in the current study, the surface effects on the vibration of the piezoelectric nanobeam will be investigated with the consideration of axial boundary constrains, which have been ignored in existing studies. In addition, the flexoelectric effect on the vibration behavior of a piezoelectric nanobeam will be studied using the higher order theory of

piezoelectricity.

2. Surface Effects on the Vibration of Piezoelectric Nanobeams

In this work, the vibration of a piezoelectric nanobeam with length L, thickness h and width b is studied with surface effects. As seen from Fig. 1(a), the beam is modeled as a bulk core surrounded by surface layers with negligible thickness. A Cartesian coordinate (x, y, z) is used to describe the piezoelectric beam, which is poled in z direction. An electric potential V is applied between the upper and lower surfaces of the beam with the electric boundary conditions $\Phi(h/2) = V$ and $\Phi(-h/2) = 0$. The electric field is assumed to exist only in the beam thickness direction and can be determined from the electric potential Φ as $E_z = -\partial \Phi/\partial z$. To account for the surface effects, a surface piezoelectricity model is adopted here [13, 14]. According to this model, the constitutive equations for the surface and bulk of the one-dimensional beam can be expressed as follows:

$$\sigma_x^{s} = \sigma_x^{0} + c_{11}^{s} \varepsilon_x - e_{31}^{s} E_z, \ D_x^{s} = D_x^{0},$$
(1)

$$\sigma_x = c_{11}\varepsilon_x - e_{31}E_z, \ D_z = e_{31}\varepsilon_x + \kappa_{33}E_z,$$
(2)

where σ_x^s and D_x^s are surface stress and surface electric displacement; σ_x^0 and D_x^0 are residual surface stress and surface electric displacement; c_{11}^s and e_{31}^s are surface elastic and piezoelectric constants; σ_x and D_z are bulk stress and bulk electric displacement; c_{11} , e_{31} and κ_{33} are bulk elastic, piezoelectric and dielectric constants; ε_x and E_z are the strain and electric field.



Figure 1. (*a*) Cross sectional view of a piezoelectric nanobeam with surface layers and bulk core. (b) An incremental element of the beam

The existence of surface stress induces traction jumps exerting on the bulk of the beam, as shown in Fig. 1(b). It should be mentioned that these traction jumps exist on the circumferential surfaces of the beam. According to the generalized Young-Laplace equations [21], traction jumps T_x and T_z can be written as:

$$T_x = \frac{\partial \sigma_x^s}{\partial x}, \ T_z = \frac{\sigma_x^s}{R}, \tag{3}$$

with R being the radius of curvature defined positively when the normal of surface is pointed towards the center of curvature. Based on the free-body diagram of an incremental element of the beam, as shown in Fig. 1(b), the governing equations of the piezoelectric nanobeam are derived as follows:

$$\frac{\partial P}{\partial x} + \int_{c} T_{x} dc = \rho b h \frac{\partial^{2} u_{0}(x,t)}{\partial t^{2}}, \qquad (4)$$

$$\frac{\partial^2 M}{\partial x^2} - P \frac{\partial^2 w(x,t)}{\partial x^2} - \int_c T_z dc - \frac{\partial \int_c T_x z dc}{\partial x} = -\rho bh \frac{\partial^2 w(x,t)}{\partial t^2},$$
(5)

where c is the perimeter of the beam cross-section; ρ is the mass density; $P = \int \sigma_x dy dz$ and

 $M = -\int \sigma_x z dy dz$ are the axial force and bending moment; $u_0(x, t)$ and w(x, t) are the axial displacement at z=0 and the transverse displacement.

Assuming that the beam thickness is much smaller than the radius of curvature induced by the applied loads and the beam cross section is constant along its length, thus, the Euler-Bernoulli beam theory can be adopted for modeling the piezoelectric nanobeam and the axial strain is expressed as:

$$\varepsilon_{x} = \frac{\partial u_{0}(x,t)}{\partial x} - z \frac{\partial^{2} w(x,t)}{\partial x^{2}}.$$
(6)

It is worth noting that in existing studies of both elastic and piezoelectric nanobeams, $u_0(x, t)$ was assumed as zero based on the conventional Euler-Bernoulli model, therefore, the first term of Eq. (6) was ignored accordingly [10-12, 14, 15]. However, this assumption may not be accurate since $u_0(x, t)$ is not necessary zero for the nanobeam with surface effects. For example, the existence of surface stress induces an axial relaxation displacement as discussed in literature [22]. In addition, for piezoelectric nanobeams, the applied electrical load may also induce an axial displacement due to the inherent electromechanical coupling of piezoelectric materials. In fact, the beam can be either constrained without axial movement or allowed to have free movement with traction free boundary conditions. Therefore, the axial boundary conditions may influence the surface effects on the vibration behavior of piezoelectric nanobeams, which will be discussed later in this section.

In the absence of free electric charges, the electric displacement satisfies Gauss's law $\partial D_x / \partial x + \partial D_y / \partial y + \partial D_z / \partial z = 0$, which gives an explicit expression of the electric field. Assuming

 $u_0(x,t)$ is independent of time *t* and substituting Eqs. (1)-(3) and (6) into Eqs. (4) and (5), the following governing equations can be obtained as:

$$\left[c_{11}bh + (2b+2h)c_{11}^{s}\right]\frac{\partial^{2}u_{0}(x)}{\partial x^{2}} = 0, \qquad (7)$$

$$(EI)^* \frac{\partial^4 w(x,t)}{\partial x^4} - N^* \frac{\partial^2 w(x,t)}{\partial x^2} = -\rho bh \frac{\partial^2 w(x,t)}{\partial t^2}, \qquad (8)$$

in which $(EI)^* = (c_{11} + e_{31}^2 / \kappa_{33})bh^3 / 12 + (c_{11}^s + e_{31}^s e_{31} / \kappa_{33})(h^3 / 6 + bh^2 / 2)$ is the effective bending rigidity of the beam and $N^* = [c_{11}\partial u_0 / \partial x + e_{31}V / h]bh + 2[\sigma_x^0 + c_{11}^s \partial u_0 / \partial x + e_{31}^s V / h]b$.

In this work, the vibration analysis will be conducted for cantilever (C-F), simply-supported (S-S)

and clamped-clamped (C-C) piezoelectric nanobeams, respectively. The boundary conditions are prescribed as:

$$u_0 = w = \frac{\partial w}{\partial x} = 0 \text{ at } x = 0, \ P^* = M^* = Q^* = 0 \text{ at } x = L \ \text{(C-F)},$$
 (9)

$$\begin{cases} u_0 = w = M^* = 0 \text{ at } x = 0 \text{ and } x = L \text{ (Case 1)} \\ P^* = w = M^* = 0 \text{ at } x = 0 \text{ and } x = L \text{ (Case 2)} \end{cases}$$
(S-S), (10)

$$u_0 = w = \frac{\partial w}{\partial x} = 0 \text{ at } x = 0 \text{ and } x = L \quad (C-C),$$
 (11)

where $P^* = \int \sigma_x dy dz + \int \sigma_x^s dc = [c_{11}\partial u_0 / \partial x + e_{31}V / h]bh + 2[\sigma_x^0 + c_{11}^s \partial u_0 / \partial x + e_{31}^s V / h](b+h)$ is the effective axial force; $M^* = (EI)^* \partial^2 w / \partial x^2$ is the effective moment; and $Q^* = (EI)^* \partial^3 w / \partial x^3 - N^* \partial w / \partial x$ is the effective shear force. It should be mentioned that two different axial boundary conditions may apply for simply-supported piezoelectric beam, as shown from Eq. (10). The beam is constrained without axial moving under the Case 1 boundary condition while traction free is adopted under the Case 2 boundary condition. The traction free boundary condition is also adopted for the cantilever Under this indicated in Eq. (9). condition, an beam as uniform strain $\varepsilon = \partial u_0 / \partial x = -\left[e_{31}Vb + 2\sigma_x^0(b+h) + 2e_{31}^sV(b+h)/h\right] / \left[c_{11}bh + 2c_{11}^s(b+h)\right]$ is induced by the applied electrical load and surface effects, which will influence the vibration behavior of piezoelectric nanobeams. After applying these boundary conditions, the resonant frequencies of the piezoelectric nanobeams can be determined. For conciseness, the derivation procedures are omitted here.

To show the surface effects on the vibration behavior of a piezoelectric nanobeam quantitatively, PZT-5H is taken as an example material with the bulk material properties being $c_{11}=126$ GPa, $e_{31}=-6.5$ C/m² and $\kappa_{33}=1.3\times10^{-8}$ C/V·m. In addition, the surface properties are taken as $c_{11}^{s}=7.56$ N/m, $e_{31}^{s}=-3\times10^{-8}$ C/m and $\sigma_{x}^{0}=1.0$ N/m. In the current work, only the first mode

resonant frequency of the piezoelectric nanobeam is studied. Firstly, the variation of the normalized resonant frequency ω^{s}/ω^{0} of a simply-supported piezoelectric nanobeam with beam thickness h under both Case 1 and Case 2 axial boundary conditions is plotted in Fig. 2. ω^0 is the resonant frequency calculated without the consideration of surface effects and the applied electrical load. The beam geometry is set as b=h and L=10h. It is clearly seen from this figure that the axial boundary constraint has a significant influence on the vibration of the piezoelectric nanobeam, as evidenced by the dissimilar variation trends. For example, when the axial boundary constraint is set as described in Case 1, the combined effects of surfaces and electrical load increase the resonant frequency of the piezoelectric nanobeams. When V=-0.1 V, the influence is the largest (ω^{s} / ω^{0} is about 1.2 at *h*=10 nm). However, under Case 2 boundary constraint, the resonant frequency can be either enhanced or reduced by the surface effects and the applied electrical load ($\omega^{\rm s}/\omega^{\rm 0}$ is about 1.01 and 0.95 when V=0.1 V and -0.1 V, respectively at h=10 nm). It is noted that the variation of resonant frequency with the applied electric potential in this figure indicates a possible avenue for frequency tuning of piezoelectric nanobeams. It is also observed that the surface effects have more prominent influence on the resonant frequency of a beam with smaller thickness. While such surface effects decrease with the increase of beam thickness h. Fig. 3 shows the variation of the normalized resonant frequency of a piezoelectric nanobeam against the beam thickness. The beam has the same geometric parameters as the one in Fig. 2 without any applied electrical load. It

demonstrates that the surface effects on the resonant frequencies of piezoelectric nanobeams are significantly influenced by the beam boundary conditions. For the S-S beam with Case 1 boundary constraint and the C-C beam, surface effects increase the resonant frequencies, while the trend is opposite for the S-S beam with Case 2 boundary constraint and the C-F beam. Again, surface effects are more significant for the beam with smaller thickness h and reduce with the increase of h. From these two figures, it is conduced that the axial boundary condition plays a substantial role in the transverse vibration of piezoelectric nanobeams with surface effects. Therefore, it is essential to consider the axial boundary constraints in predicting the vibration behavior of piezoelectric nanobeams.



Figure 2. The normalized resonant frequency ω^s / ω^0 versus beam thickness *h* for a simply-supported piezoelectric nanobeam with surface effects under different axial boundary conditions



Figure 3. The normalized resonant frequency ω^{s} / ω^{0} versus beam thickness *h* for a piezoelectric nanobeam with surface effects under different boundary conditions

As mentioned before, the applied electrical load and surface effects will induce an axial strain when the axial traction free condition is prescribed for the beam. As shown in Fig. 4, without the consideration of the surface effects, the product of this axial strain with the beam thickness is a constant, i.e., $\varepsilon h = -e_{31}V/c_{11}$. When V=0 V, no axial strain is induced for the beam without considering the surface effects. However, the existence of the residual surface stress will still induce a relaxation strain as shown by the curve V=0 V with surface effects in Fig. 4. This relaxation phenomenon has been well discussed in [22] based on atomistic simulations. It is also observed in this figure that the surface effects lead to the size-dependency of this axial strain.



Figure 4. Axial strain εh versus beam thickness h for a piezoelectric nanobeam under different applied electrical load

3. Flexoelectricity on the Vibration of Piezoelectric Nanobeams

Flexoelectricity is induced by non-uniform deformation or strain gradient, which becomes significant as the structural size scales down to nanometers. To account for this effect, the higher order theory of piezoelectricity incorporating the strain gradient term will be adopted in the current work for a C-C beam. The same Cartesian coordinate system as shown in Fig. 1 is used to describe a piezoelectric nanobeam with flexoelectricity. The geometry, poling direction and electric boundary conditions of the beam are the same as those stated in Section 2. Under Euler-Bernoulli assumption, the axial strain can be defined as $\varepsilon_x = -z\partial^2 w/\partial x^2$. In the current study, we only consider the strain gradient $\varepsilon_{x,z}$, while $\varepsilon_{x,x}$ is ignored due to the large length scale along the beam axis direction. The relevant stress and electric field are σ_x and E_z , which can be expressed as [18]:

$$\sigma_x = c_{11}\varepsilon_x + d_{31}P_z, \ E_z = a_{33}P_z + d_{31}\varepsilon_x + f_{13}\varepsilon_{x,z},$$
(12)

where P_z is polarization; a_{33} is dielectric susceptibility; and f_{13} is the flexoelectric coefficient. In addition, a higher order stress $\sigma_{xxz} = f_{13}P_z$ is introduced in the piezoelectricity theory. In the absence of free surface charges, the Gauss's law can be written as:

$$-\varepsilon_0 \frac{\partial^2 \Phi}{\partial z^2} + \frac{\partial P_z}{\partial z} = 0, \qquad (13)$$

where $\varepsilon_0 = 8.85 \times 10^{-12}$ F/m is the dielectric permittivity of a vacuum. From Eqs. (12) and (13) with the consideration of electric boundary conditions of the beam, the polarization in the piezoelectric beam can be determined as:

$$P_{z} = \frac{\varepsilon_{0}d_{31}}{\varepsilon_{0}a_{33}+1} z \frac{\partial^{2}w(x,t)}{\partial x^{2}} + \frac{f_{13}}{a_{33}} \frac{\partial^{2}w(x,t)}{\partial x^{2}} - \frac{V}{a_{33}h}.$$
(14)

It is clearly seen from this equation that polarization can be induced by flexoelectricity. The governing equation of the flexoelectric nanobeam is formulated from Hamilton's principle [18]: $\delta U - \delta T - \delta W = 0, \qquad (15)$

where $U = \frac{1}{2} \int_{t_1}^{t_2} \int_{\Pi} \left(\sigma_x \varepsilon_x + \sigma_{xxz} \varepsilon_{x,z} \right) d\Pi dt$ (*t* is the time and Π is the entire domain of the structure) is the strain energy, and $T = \frac{1}{2} \int_{t_1}^{t_2} \int_{\Pi} \rho \left(\frac{\partial w}{\partial t} \right)^2 d\Pi dt$ is the kinetic energy. The resultant axial force is

defined as $P_x = b \int_{-h/2}^{h/2} (\sigma_x - \sigma_{xxz,z}) dz$, with the consideration of applied shear force Q_0 , Q_L and moment M_0 , M_L , the work is defined as $W = -\frac{1}{2} \int_{t_1}^{t_2} \left[\int_0^L P_x \left(\frac{\partial w}{\partial x} \right)^2 dx + M_L \frac{\partial w}{\partial x} \Big|_L - M_0 \frac{\partial w}{\partial x} \Big|_0 - Q_L w_L + Q_0 w_0 \right] dt_0$. With these defined quantities,

the governing equation is derived from Eq. (15) as:

$$A^* \frac{\partial^4 w(x,t)}{\partial x^4} + \frac{d_{31}}{a_{33}} V b \frac{\partial^2 w(x,t)}{\partial x^2} = -\rho b h \frac{\partial^2 w(x,t)}{\partial t^2}, \qquad (16)$$

with $A^* = \left[c_{11} - \varepsilon_0 d_{31}^2 / (\varepsilon_0 a_{33} + 1)\right] bh^3 / 12 - f_{13}^2 / a_{33} bh$.



Figure 5. The normalized resonant frequency $\omega^{\text{flexo}} / \omega^0$ versus beam length to thickness ratio L/h for a piezoelectric nanobeam with flexoelectricity

For case study, the vibration of a clamped-clamped (C-C) piezoelectric nanobeam is investigated with the consideration of flexoelectricity. BaTiO₃ is taken as the example material with material properties being $c_{11} = 167.5$ GPa, $d_{31} = 3.5 \times 10^8$ V/m and $a_{33} = 0.8 \times 10^8$ V·m/C. The flexoelectric coefficients of BaTiO₃ can be determined from experiments or atomistic simulations. Following Ref. [19], in which the typical value of the flexoelectric coefficient is 1–10 V, we take $f_{13} = 5$ V. The variation of the normalized resonant frequency $\omega^{\text{flexo}} / \omega^0$ of the piezoelectric nanobeam against the beam length to thickness ratio L/h is plotted in Fig. 5, in which ω^0 is the resonant frequency calculated without the consideration of flexoelectricity and applied electrical load. The beam length is L=500 nm and b/h=1. When the applied electric potential is V=0 V, it is seen that flexoelectricity decreases the resonant frequency of the clamped-clamped beam and this influence increases with the increase of L/h. The size-dependency of flexoelectricity is clearly demonstrated in this figure and such effect becomes negligible when the beam thickness becomes large, for example, the results with the consideration of the flexoelectricity approach to those from the classical theory when L/h=5. It is also observed that the influence of flexoelectricity on the normalized resonant frequency of the piezoelectric nanobeam depends on applied electrical load, as evidenced by the discrepancies among the results under different applied electrical load, which again indicate the possible frequency tuning of piezoelectric nanobeams must incorporate the influence of flexoelectricity.

4. Conclusions

The influence of surface effects and flexoelectricity on the vibration behavior of piezoelectric nanobeams is investigated in the current work. Surface effects are incorporated into the modeling through the surface piezoelectricity model and the generalized Young-Laplace equations. In addition to the transverse boundary conditions, the axial boundary constraints are also considered for the beam with surface effects. Simulation results indicate both axial and transverse boundary constraints significantly influence the surface effects on the resonant frequencies of piezoelectric nanobeams. An axial strain relaxation is also observed under axial traction free boundary condition. Both applied electrical load and surface effects will affect such a relaxation phenomenon. Flexoelectric effect also has a substantial effect on the vibration of piezoelectric nanobeams. Both surface effects and the effect of flexoelectricity are more prominent for piezoelectric nanobeams with smaller thickness, which are attributed to the size-dependent properties of piezoelectric nanobeams. It is also observed that the resonant frequencies can be tuned by adjusting the applied electrical load. This work is expected to provide a better physical understanding of piezoelectric nanobeams and a guideline for the design of piezoelectric nanobeam-based devices.

Acknowledgements

This work was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC).

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