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Study the Postbuckling of Hexagonal Piezoelectric Nanowires with Surface Effect

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Abstract

Piezoelectric nanobeams having circular, rectangular and hexagonal cross-sections are synthesized and used in various Nano structures; however, piezoelectric nanobeams with hexagonal cross-sections have not been studied in detail. In particular, the physical mechanisms of the surface effect and the role of surface stress, surface elasticity and surface piezoelectricity have not been discussed thoroughly. The present study investigated post-buckling behavior of piezoelectric nanobeams by examining surface effects. The energy method was applied to post-buckling of hexagonal nanobeams and the critical buckling voltage and amplitude are derived analytically from bulk and surface material properties and geometric factors.

1. Introduction

Nano beams and Nano plates play important roles in sensing and actuation of nano-electromechanical systems in different fields of engineering. Piezoelectric nanobeams are promising for a range of applications in nanotechnology, such as nanosensors/transducers, nano-resonators, diodes and piezoelectric field-effect transistors [1] .

Studies on the influence of surface effects on the electromechanical behavior of piezoelectric elements include that of Chen et al. [2], who analyzed Young's modulus size-dependency in nanowires made with ZnO. Wang and Feng [3] studied the influence of surface effects on the buckling of nanobeams under axial compression. Xiang et al. [4] investigated piezoelectricity in ZnO nanobeams. Zhao et al. [5] examined the piezoelectric properties of nano-belts using a piezoresponse force microscope. Gurtin et al. [6] developed a model based on surface elasticity and residual surface stress using the Young-Laplace equation. Lilly and He [7] studied the bending of nanowires (NWs) based on the Euler-Bernoulli beam model. In recent years, the mechanical behavior of nano-elements has been of interest in response to developments in nanotechnology. Yan and Jiang [8] presented an analytical model to study vibration and buckling of nano-sized beams considering surface effects. They [9] investigated the influence of surface effects on the electromechanical coupling and bending behavior of piezoelectric nanobeams. The surface effects considered were surface elasticity and surface piezoelectricity [10].

The present study examined the influence of surface stress on post-buckling of NWs with hexagonal cross-sections using the energy method using an analytical solution for the clamped-clamped boundary condition.

2. Analytical Formulation

The current work was conducted on a piezoelectric nanobeam with a hexagonal cross-section [11]. Figure 1 depicts the piezoelectric clamped-clamped nanobeam.

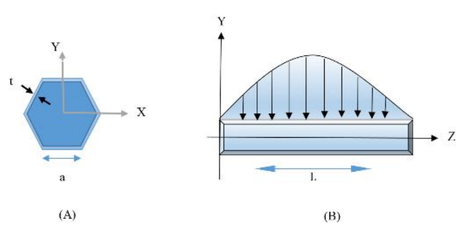

Fig. 1. (A) The hexagonal cross-section with surface layer (B) schematic diagram of nanowire

Axial strain (ε_{zz}) at any point on the beam can be defined as:

$$\varepsilon_{zz} = \varepsilon_0 + \kappa y \tag{1}$$

where ε_0 is the strain component of the mid-plane and k is the curvature of the surface caused by buckling or bending. The electrical field is assumed to exist only in the y direction. Electrical field E_y is related to electric potential ϕ as:

$$E_y = -\frac{\partial \phi}{\partial y} \tag{2}$$

The constitutive relations in the bulk piezoelectric materials can be defined as:

$$\sigma_{zz} = \bar{\mathrm{E}}\varepsilon_{zz} - \bar{e}E_y \tag{3}$$

$$D_y = \bar{e}\varepsilon_{zz} + \bar{k}E_y \tag{4}$$

where σ_{zz} is the axial stress, D_y is the electrical displacement, and $\bar{\mathrm{E}}$, $\bar{e}$ and $\bar{k}$ are the elastic, piezoelectric and dielectric constants.

Huang and Yu [12] used constitutive equations for the surface of a beam as:

$$\sigma_{zz}^s = \sigma_{zz}^0 + \bar{\mathrm{E}}^s\varepsilon_{zz} - \bar{e}^s E_y \tag{5}$$

$$D_y^s = D_y^0 + \bar{e}^s \varepsilon_{zz} + \bar{k}^s E_y \tag{6}$$

where σ_{zz}^s is the surface stress and D_y^s is the surface electric displacement, $\bar{\mathrm{E}}^s$, $\bar{e}^s$ and $\bar{k}^s$ are the surface elastic, surface piezoelectric and surface dielectric constants, σ_{zz}^0 is the surface stress and D_y^0 is the surface electric displacement. In the absence of free electrical charges, the dielectric governing equation is:

$$\frac{\partial D_y}{\partial y} = 0 \tag{7}$$

Using $\phi\left(-\frac{\sqrt{3}}{2}a\right)=0$, $\phi\left(-\frac{\sqrt{3}}{2}a\right)=0$ and $\phi\left(\frac{\sqrt{3}}{2}a\right)=V$ in Equations (2), (4) and (7) gives:

$$\phi(y)=\frac{\bar{e}\kappa}{2\bar{k}}y^{2}+\frac{V}{a\sqrt{3}}y+Constant \tag{8}$$

The electrical potential of the rectangular cross-section was applied to the model. Using Equation (2), the electrical field can be expressed as:

$$E_{y}=-\frac{V}{a\sqrt{3}}-\frac{\bar{e}\kappa}{\bar{k}}y \tag{9}$$

Using Equation (9), constitutive Equations (3), (4), (5) and (6) for the piezoelectric nanobeam can be rewritten as:

$$\sigma_{zz}=\bar{\mathrm{E}}\left(\varepsilon_{0}+\frac{\bar{e}V}{\bar{\mathrm{E}}a\sqrt{3}}\right)-\bar{\mathrm{E}}\left(1+\frac{\bar{e}^{2}}{\bar{k}\bar{\mathrm{E}}}\right)\kappa y \tag{10}$$

$$D_{y}=\bar{e}\varepsilon_{0}-\frac{\bar{k}V}{a\sqrt{3}} \tag{11}$$

$$\sigma_{zz}^{s}=\sigma_{zz}^{0}+\bar{\mathrm{E}}^{s}\left(1+\frac{\bar{e}\bar{e}^{s}}{\bar{k}\bar{\mathrm{E}}}\right)\kappa y-\bar{\mathrm{E}}^{s}\left(\varepsilon_{0}+\frac{\bar{e}^{s}V}{\bar{\mathrm{E}}^{s}a\sqrt{3}}\right) \tag{12}$$

$$D_{y}^{s}=D_{y}^{0}+\bar{e}^{s}\varepsilon_{0}-\frac{\bar{k}^{s}V}{a\sqrt{3}} \tag{13}$$

For hexagonal cross-section, bending rigidity (EI) and tensile rigidity can be derived as:

$$(EI)_{eff}=\frac{5\sqrt{3}}{16}a^{4}\bar{\mathrm{E}}\left(1+\frac{\bar{e}^{2}}{\bar{k}\bar{\mathrm{E}}}\right)+\dots \\ \dots+\frac{5}{2}a^{3}\bar{\mathrm{E}}^{s}\left(1+\frac{\bar{e}\bar{e}^{s}}{\bar{k}\bar{\mathrm{E}}}\right) \tag{14}$$

$$(EA)_{eff}=\frac{3\sqrt{3}}{2}a^{2}\bar{\mathrm{E}}\left(1+\frac{\bar{e}V}{\bar{\mathrm{E}}a\varepsilon_{0}\sqrt{3}}\right)+\dots \\ \dots+6a\bar{\mathrm{E}}^{s}\left(1+\frac{\bar{e}^{s}V}{\bar{\mathrm{E}}^{s}a\varepsilon_{0}\sqrt{3}}\right) \tag{15}$$

It was assumed that the top and bottom surfaces have residual surface tension σ_{zz}^{0}. The Laplace-Young equation [13] gives the distributed loading on the two surfaces as:

$$p(z)=2a\sigma_{zz}^{0}w_{,zz} \tag{16}$$

where $w_{,zz}$ is the second derivation of beam deflection with respect to z (Figure 1). The energy method was used to study the post-buckling behavior of the piezoelectric nanobeam. Elastic nonlinear von Karman beam assumptions were applied in this method. The total energy is [14]:

$$U_{total}=U_{m}+U_{b}+U_{e}+U_{r} \tag{18}$$

where U_{m} is the membrane energy, U_{b} is the bending energy, U_{e} is the negative electric energy and U_{r} is the energy related to surface residual energy.

The clamped-clamped boundary condition was assumed, i.e., $w=0$, $w_{,z}=0$ at $z=0,L$. The boundary conditions are satisfied by the following beam deflection:

$$w=Amp\left(1-\cos\left(\frac{2\pi}{L}z\right)\right) \tag{19}$$

where amplitude (Amp) can be obtained by energy minimization and w is the out-of-plane displacement of the nanobeam. The displacement-strain relation is:

$$\varepsilon_{0}=\frac{du_{z}}{dz}+\frac{1}{2}\left(\frac{dw}{dz}\right) \tag{20}$$

Membrane force N_{zz} in the beam is:

$$N_{zz}=\left(EA\right)_{eff}\ \varepsilon_0$$

$$N_{zz}=\frac{3\sqrt{3}}{2}a^2\bar{\mathrm{E}}\left(\varepsilon_0+\frac{\bar{e}V}{\bar{\mathrm{E}}a\sqrt{3}}\right)+\ldots \qquad (21)$$
$$\ldots+6a\bar{\mathrm{E}}^s\left(\varepsilon_0+\frac{\bar{e}^sV}{\bar{\mathrm{E}}^sa\sqrt{3}}\right)$$

Force equilibrium $\frac{dN_{zz}}{dz}=0$ requires the membrane force to be constant; consequently, the membrane strain is constant.

The substitution of Equation (19) into Equation (20) results in the in-plane displacement: $u_z=\frac{Amp^2\pi}{2L}\sin\left(\frac{4\pi}{L}z\right)$

(22)

Substituting Equation (22) and (19) into Equation (20) results in:

$$\varepsilon_0=\frac{2\pi^2Amp}{L^2}cos^2\left(\frac{2\pi}{L}z\right) \qquad (23)$$

The membrane energy in the beam can be obtained as:

$$U_m=\int_0^L\frac{1}{2}\left(EA\right)_{eff}\ {\varepsilon_0}^2dz=$$
$$\frac{3\pi^4Amp^4}{4L^3}\left(\frac{3\sqrt{3}a^2\bar{\mathrm{E}}}{2}+6a\bar{\mathrm{E}}^s\right)+\ldots \qquad (24)$$
$$\ldots+\frac{\pi^2Amp^2}{2L}\left(\frac{3a\bar{e}V}{2}+\frac{6\bar{e}^sV}{\sqrt{3}}\right)$$

The bending energy becomes:

$$U_b=\int_0^L\frac{1}{2}\left(EI\right)_{eff}\ (\frac{\partial^2w}{\partial z^2})^2dz=$$
$$4\begin{pmatrix}\frac{5\sqrt{3}}{16}a^4\bar{\mathrm{E}}\left(1+\frac{\bar{e}^2}{\bar{k}\bar{\mathrm{E}}}\right)+\ldots\\ \ldots+\frac{5}{2}a^3\bar{\mathrm{E}}^s\left(1+\frac{\bar{e}\bar{e}^s}{\bar{k}\bar{\mathrm{E}}}\right)\end{pmatrix}\left(\frac{Amp^2\pi^4}{L}\right) \qquad (25)$$

Negative electrical energy in the beam is a response to the residual surface electrical displacement, surface module and surface electric displacement and can be obtained as:

$$U_e=-a\int_0^L\int_{-a\sin(60)}^{a\sin(60)}\frac{D_yE_ydydz}{2}$$
$$=\frac{V}{6L}(3Amp^2\pi^2a\bar{e}-\bar{k}V\sqrt{3}L^2) \qquad (26)$$

Surface residual stress energy U_r is:

$$U_r=-\frac{1}{2}\int_0^Lp\left(z\right)w\left(z\right)dz$$
$$=\frac{2a\sigma_{zz}^0Amp^2\pi^2}{L} \qquad (27)$$

Total energy U_{total} is the sum of the bending, membrane, electrical and surface residual stress energies. Minimization of U_{total} with respect to Amp gives:

$$Amp=\left(\frac{L}{3}\right)\left(\frac{\sqrt{-a\bar{E}\bar{k}\left(3a\bar{E}+4\bar{E}^s\sqrt{3}\right)}}{\pi a\bar{E}\bar{k}\left(3a\bar{E}+4\bar{E}^s\sqrt{3}\right)}\right)\sqrt{X}$$

(28-a)

Where X is expressed as:

$$X=(15\bar{E}^2\pi^2a^4\bar{k}+40\bar{E}\bar{E}^s\sqrt{3}\pi^2a^3\bar{k}$$
$$+15\bar{E}\pi^2a^4\bar{e}^2+40\bar{E}^s\sqrt{3}\pi^2a^3\bar{e}\bar{e}^s+$$
$$+5\bar{E}\sqrt{3}Va\bar{e}\bar{k}+8\bar{E}\sqrt{3}a\bar{k}\sigma_{zz}^0+12\bar{E}V\bar{e}^s\bar{k}$$

(28-b)

Critical voltage can then be from the amplitude as:

$$V=-\frac{a\left(15\bar{E}^2\pi^2a^3\bar{k}+40\bar{E}\bar{E}^s\sqrt{3}\pi^2a^2\bar{k}+15\bar{E}\pi^2a^3\bar{e}^2\right)}{\bar{E}\bar{k}\left(5\sqrt{3}a\bar{e}+12\bar{e}^s\right)}+$$
$$+\frac{a(40\bar{E}^s\sqrt{3}\pi^2a^2\bar{e}\bar{e}^s+8\bar{E}\sqrt{3}a\bar{k}\sigma_{zz}^0)}{\bar{E}\bar{k}\left(5\sqrt{3}a\bar{e}+12\bar{e}^s\right)}$$

(29)

Neglecting the surface effect and substituting $\sigma_{zz}^0=0$, $\bar{\mathrm{E}}^s=0$ and $\bar{e}^s=0$ into

Equations (28) and (29) normalizes V and Amp. Amp and V without surface effects becomes:

$$A_0 = \frac{L\sqrt{-3\bar{k}(15\bar{E}\pi^2 a^4\left(\bar{k}\bar{E}+\bar{e}^2\right)+5\sqrt{3}\ \bar{E}Va\bar{e}\bar{k})}}{9\pi\bar{E}\bar{k}a} \tag{30}$$

$$V_{cr}^{0} = -\frac{\sqrt{3}a^3\pi^2\left(\bar{E}\bar{k}+\bar{e}^2\right)}{\bar{e}\bar{k}} \tag{31}$$

3. Results and discussion

The present study investigated the influence of surface effects on the post-buckling behavior of PZT hexagonal and rectangular nanobeams. The bulk properties of PZT were assumed to be $e = -5.02C/m^2$, $E = 95\ GPa$, and $K = 3.3\times10^{(-9)} F/m$ [10]. The surface properties were $\sigma_{zz}^{0} = 1N/m$, $\bar{E}^{s} = 7.56N/m$ and $\bar{e}^{s} = -3\times10^{-8} C/m$ [8]. The length-to-thickness ratio of the piezoelectric NWs was set at 40.

The hexagonal cross-section was considered to be surrounded by a rectangle with a height of $2\times a\times sin\left(\frac{\pi}{3}\right)$. Equation (32) was used to normalize the critical voltage. The normalized critical voltage $(Vcr/Vcr0)$ versus the thickness h of the rectangular and side a of the hexagonal piezoelectric nanowires are shown in figures 2 and 3.

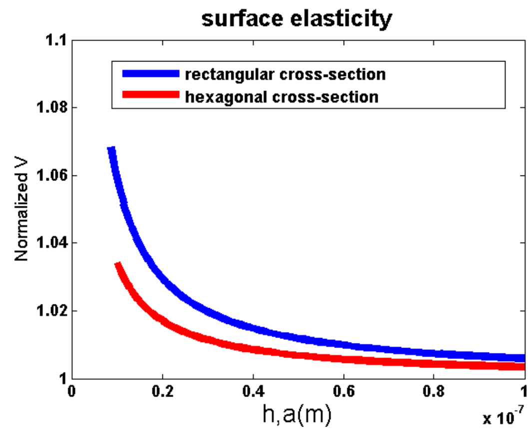

Fig. 2. The normalized critical voltage with surface elasticity versus the thickness h and side a.

To study surface elasticity, $\bar{e}^{s} = 0$, $\sigma_{zz}^{0} = 0$ and $\bar{E}^{s} \neq 0$ were assumed. To show the surface piezoelectricity, the surface properties were assumed to be $\bar{e}^{s} = 0$, $\sigma_{zz}^{0} \neq 0$, and $\bar{E}^{s} = 0$. The value of h and a were assumed 10 nm to 100 nm.

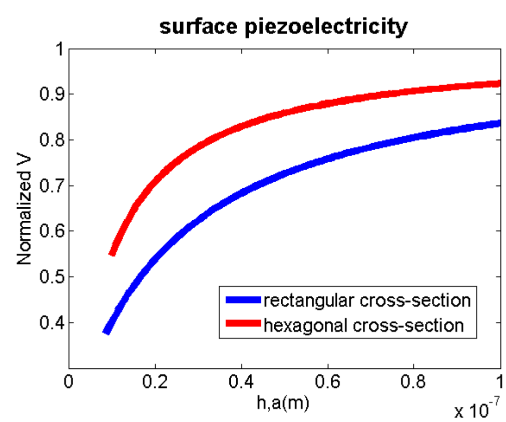

Fig. 3. The normalized critical voltage with surface piezoelectricity versus the thickness h and side a.

Figures 2 and 3 indicate that, when a and h are greater than 100 nm, the normalized critical voltage tends to remain constant. Figure 2 shows that increasing h and a decreased the normalized critical voltage in both cross-sections. Figure 3 shows that the normalized critical voltage increased as h and a increased.

The assumptions made in the present study correspond to those of previous research; modifications in the cross-section were made to provide reasonable comparison with previous work. The cross-section was assumed to be rectangular and the hexagonal cross-section was assumed to be surrounded by a rectangle. To validate the proposed model, the results are compared with results from Li et al. [14] (Table 1). The table shows the normalized amplitude versus V/V_{cr} with and without surface effect. As shown, the results are remarkably similar.

Table 1. Normalized amplitude versus V/V_{cr}

V/V_{cr}		A/A_0 Rectangular Li et al. [14]	A/A_0 Hexagonal [Present]
5	With surface effect	2.46559	2.07754
	Without surface effect	2.23607	2.0000
6	With surface effect	2.70443	2.33576
	Without surface effect	2.44949	2.23607
7	With surface effect	2.9238	2.56815
	Without surface effect	2.64575	2.44949
8	With surface effect	3.12787	2.78118
	Without surface effect	2.82843	2.64575
9	With surface effect	3.31939	2.97902
	Without surface effect	3.00000	2.82843

The cross-section was assumed to be circular and the hexagonal cross-section was assumed to be surrounded by a circular. To validate the proposed model, the results are compared with results from Wang et al. [3] (Table 2).

4. Conclusion

The piezoelectric response of piezoelectric nanobeams is a topic of recent research where continuum piezoelectric theory is efficiently used as a cost effective technique. The present study was an analytical approach to study post-buckling of piezoelectric hexagonal nanobeams caused by an electrical field considering surface effects and critical voltage.

Table 2. The critical compressive load of axial buckling of nanowire

Pcr/Pcr0	L/D=20	
D=2a	Hexagonal [Present]	Circular Wang et al. [3]
80	1.17	1.96
100	1.14	1.77
120	1.11	1.64
140	1.10	1.55
160	1.08	1.48
180	1.07	1.43
200	1.07	1.38

The results showed that surface effects should be considered when the beam thickness decreases to nano-size. The model was used to investigate the surface effect on critical buckling voltage and its dependence on the geometric size of the piezoelectric nanobeams. The proposed approach can be a theoretical basis for the accurate design of piezoelectric nanostructures in future studies.

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