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Surface effects on the post-buckling of piezoelectric nanowires

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HIGHLIGHTS

- A continuum energy model is developed to investigate the surface effects on postbuckling of piezoelectric nanowires.
- The critical postbulking strain and amplitude are obtained under open electric circuit condition.
- Theoretical results agree well with the experiment data.

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ABSTRACT

Due to the large ratio of surface to volume, surface effects play an essential role in determining the physical properties of nanoscaled structures. A theoretical model is developed in this work to investigate the effect of surface on the postbuckling behavior of piezoelectric nanowires, in which the residual surface stresses, surface piezoelectricity and surface elasticity are taken into consideration. The critical buckling strain and the amplitude of the buckled nanowire are analytically obtained. It is found that the critical buckling strain ratio increase with the decrease of the thickness of piezoelectric nanowire, which demonstrates that the surface becomes prominent when the thickness of piezoelectric nanowire is at nano-scale. The theoretical estimation agrees well with the experimental data on a single crystal ZnO nanowire. This study provided the fundamental understanding of the physical behavior of piezoelectric nanowires and is promising for designing piezoelectric nanowire based stretchable nanoelectronics.

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1. Introduction

One dimensional (1D) nanostructures such as nanobelts, nanowires and nanorings are one of the most important nanostructures due to their promising applications as sensors, transistors, self-powered nanogenerator and scanning probe microscopy [1–3]. Unlike the macroscopic physical properties, nanowires show size-dependent physical and mechanical properties due to the large ratio of surface to volume [4]. It is widely accepted that the surface plays a key role in the electromechanical coupling behavior of piezoelectric nanowires.

The investigation on the surface effects on the mechanical behavior of nanowires have been performed based on the surface elasticity theory [5,6]. The generalized Young–Laplace equation of curved interfaces in nanoscaled solids was derived by Chen et al. [7]. The effect of surface elasticity on the effective properties was constructed in a simple sample and the results were compared with the predictions by atomistic simulation, it is found that the effective stiffness properties of nanosized structural elements differ from those predicted by standard continuum mechanics [8]. The surface properties and effective properties of silver nanowires were measured by using contact atomic force microscopy and the apparent size dependent of elastic properties were analyzed [9]. The effects of residual surface tension and surface elasticity on the natural frequency and on the buckling of nanowires were analytically discussed [10,11]. And the postbuckling behavior of nanowires with surface effects has been theoretically discussed based on an energy model [12]. All the mentioned researches studied the surface effects on mechanical properties of nanowires; however, the effect of surface on the electromechanical coupling behavior of piezoelectric nanowires has not been considered.

As important fundamental elements, piezoelectric nanowires are regarded as the building blocks for energy harvesters and field effect transistors. The piezoelectric constants for ZnO nanowires have been calculated using the classical polarizable core–shell potentials [13]. A continuum theory of surface piezoelectricity for nanodielectrics was established by Pan et al. [14] to derive the modified governing equations and boundary conditions. The generalized Young–Laplace equations with surface effects for nano-dielectrics have been established by Shen and Hu [15–17]. Then the surface piezoelectricity and the emergence of

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piezoelectricity in non-piezoelectric structures have been experimentally investigated [18]. The electromechanical coupling and bending behavior of piezoelectric nanowires were analytically discussed with the consideration of the surface effects [19], while the vibration and buckling of piezoelectric nanoplate were solved with surface effects [20,21]. The critical buckling voltage of piezoelectric nanowires with the surface effects has been investigated and discussed [22]. The buckling of piezoelectric nanofilms with the effects of surface was discussed and solved [23]. The physical properties of vertical ZnO nanowires were successfully determined by using buckling characterization in nanoindentation test [24]. In view of the importance of buckling and postbuckling in nanoscale systems, it is important to study the post-buckling behavior of piezoelectric nanowires with surface effects. The objection of this paper is to develop an energy model to study the postbuckling of piezoelectric nanowires with the consideration of surface residual stresses, surface elasticity and surface piezoelectricity.

2. Piezoelectric nanowires with surface effects

The surface constitutive equations for piezoelectric materials can be expressed as [8,10,11,15,19,20,23]

$$\sigma^s_{\alpha\beta} = \Gamma_{\alpha\beta} + c^s_{\alpha\beta\gamma\kappa}\varepsilon^s_{\gamma\kappa} - e^s_{\kappa\alpha\beta}E^s_\kappa D^s_\kappa = D^0_\kappa + e^s_{\kappa\alpha\beta}\varepsilon^s_{\alpha\beta} + a^s_{\kappa\gamma}E^s_\gamma \tag{1}$$

where $c^s_{\alpha\beta\gamma\kappa}$, $e^s_{\kappa\alpha\beta}$ and $a^s_{\gamma\kappa}$ being the surface elastic, surface piezoelectric and surface dielectric constants. $\Gamma_{\alpha\beta}$ and D^0_κ are residual surface stresses and surface electric displacement without applied mechanical stimuli and electrical stimuli, respectively.

For the buckling problem of piezoelectric nanowire, one dimensional surface constitutive equation is utilized for the sake of simplicity. Eq. (1) can be rewritten as

$$\sigma^s_{xx} = \Gamma_{11} + c^s_{11}\varepsilon^s_{xx} - e^s_{31}E^s_3, \quad D^s_x = D^0_x \tag{2}$$

where the surface strain and the surface electric field are the projection of bulk strain and electric field on the surface so that $\varepsilon^s_{11} = \varepsilon_{11}|_s$ and $E^s_3 = E_3|_s$.

The one dimensional piezoelectric constitutive equations are

$$\sigma_{11} = c_{11}\varepsilon_{11} - e_{31}E_3, \quad D_3 = a_{33}E_3 + e_{31}\varepsilon_{11} \tag{3}$$

Under the open circuit condition the electric displacement $D_3 = 0$ on the beam surfaces [19] where the electrical Gauss's law satisfied naturally.

The effective flexural rigidity $(EI)_*$ and the effective tensile rigidity $(EA)_*$ can be rewritten as

$$\begin{cases} (EI)_* = (EI)_b + (EI)_s \\ (EA)_* = (EA)_b + (EA)_s \end{cases} \tag{4}$$

with $(EI)_b = (c_{11} + e^2_{31}/a_{33})I$ is the flexural rigidity of the bulk piezoelectric beam and $(EI)_s = (c^s_{11} + e_{31}e^s_{31}/a_{33})I_s$ is the flexural rigidity of the surface. $(EA)_b = (c_{11} + e^2_{31}/a_{33})A$ and $(EA)_s = (c^s_{11} + e_{31}e^s_{31}/a_{33})c_0$ are the tensile rigidity for the bulk and surface piezoelectric beam, respectively. The parameter c_0 is the length of the object line of the cross section.

When the effect of surface is taken into account, the stress jump on the surface induced by the residual surface stress should be appropriately considered as [7,15]

$$\langle \sigma^+_{ij} - \sigma^-_{ij} \rangle n_i n_j = \Gamma_{11}\kappa \tag{5}$$

where σ^+_{ij} and σ^-_{ij} are the stresses above and below the surface, κ is the curvature of the surface and n_i the unit normal vector. Without applied mechanical and electrical loading, the residual stress has no effect on the beam deformation, however, for a beam with transverse displacement $w(X)$, the curvature is approximated by

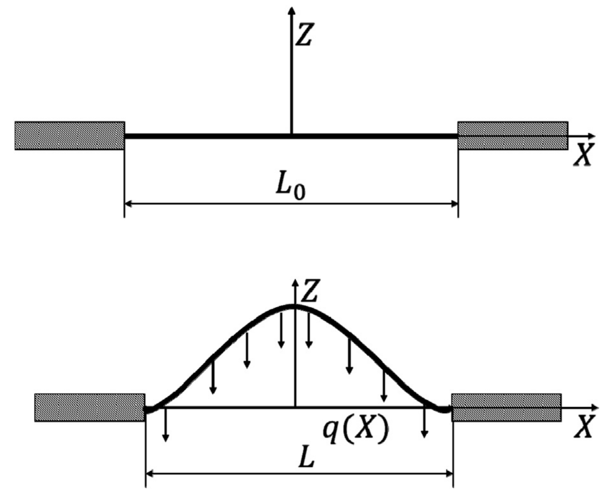

Fig. 1. Schematic of double clamped piezoelectric nanowire: (a) the undeformed piezoelectric nanowire where the residual stress self-equilibrated and (b) the buckled piezoelectric nanowire where the residual stress induces distributed transverse loading.

$\kappa \equiv \mathrm{d}^2w/\mathrm{d}x^2$ with the opposite normal vector on the upper and lower surface, the residual surface stress results in a distributed transverse loading $q(X)$ on the surface [19,21]

$$q(X) = H\frac{\mathrm{d}^2w}{\mathrm{d}x^2} \tag{6}$$

Considering a double clamped piezoelectric nanowire subjected uniaxial compression. The initial length of the nanowire is L_0 and the length becomes L after buckling (Fig. 1).

The energy model for elastic nanowire with surface elasticity and surface residual stresses was developed by Li et al. to investigate a double clamped nanowire under buckling. However, the effect of surface piezoelectricity on the buckling and post-buckling analysis of piezoelectric nanowire has not been performed. As was studied previously, surface piezoelectricity is essential to derive the effective electromechanical coupling (EMC) coefficient and it dramatically enhanced the EMC coefficient of piezoelectric nanowires [19,21]. In this study, the bending energy U_b, the surface energy U_s is modified by the bulk and surface piezoelectricity.

As in Ref. [21], the transverse displacement $w(X)$ is written as

$$w(X) = \frac{A}{2}\left(1 + \cos\frac{2\pi X}{L_0}\right) \tag{7}$$

with the boundary conditions $w|_{X=\pm L_0/2} = 0$ and $w'|_{X=\pm L_0/2} = 0$ satisfied.

When buckling occur the total energy is the sum of bending energy, tensile energy and the energy due to the surface residual stress, which are defined as

$$\begin{aligned} U_{total} &= U_b + U_t + U_r \\ &= \int_{-L_0/2}^{L_0/2} \frac{1}{2}(EI)_*\left(\frac{\mathrm{d}w}{\mathrm{d}X}\right)^2 \mathrm{d}X + \int_{-L_0/2}^{L_0/2} \frac{1}{2}(EA)_*\varepsilon_m^2\, \mathrm{d}X \\ &\quad - \int_{-L_0/2}^{L_0/2} \frac{1}{2}q(X)w\, \mathrm{d}X \end{aligned} \tag{8}$$

where the axial strain is modeled as $\varepsilon_m = \mathrm{d}u/\mathrm{d}X + (\mathrm{d}w/\mathrm{d}X)^2/2$. With the help of the axial equilibrium equation $\mathrm{d}N/\mathrm{d}X = 0$, the axial strain can be obtained as $\varepsilon_m = (\pi A^2/16L_0)\sin(4\pi X/L_0) - \varepsilon X$. Here $\varepsilon = (L_0 - L)/L_0$ is the compressive strain. Minimization the total energy with respect to the amplitude A yields that

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