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Surface and thermal load effects on the buckling of curved nanowires

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ABSTRACT

This paper investigates the impact of surface energy and thermal loading on the static stability of nanowires. We model nanowires as curved fixed–fixed Euler-Bernoulli beams and use Gurtin-Murdoch model to represent surface energy. The model takes into account both von Kármán strain and axial strain. We derive the nanowire equilibrium equations and deploy it to investigate the buckling of nanowires. We report the wire rise, critical buckling loads, and buckled wire configurations as functions of axial load in the presence of thermal loads. We found that surface energy has significant effect on the behaviour of silicon nanowires of diameter less than 4 nm. We also found that critical buckling load increases with increase in surface tensile stress and decreases with thermal loading.

1. Introduction

Nano materials have been the interest of many researchers over the past decade due to their enhanced properties. The difference in bonding forces between atoms on the surface and those in the material bulk results in changes in surface energies, mechanical, and electrical properties. For nanostructures, the surface to volume ratio is significant which gives rise to the effects of surface energy [1,2]. This surface effect includes the effects of surface stress, oxidation layer, and surface roughness which can result in increasing the elastic modulus as much as three times as that of the material bulk [3].

It has been experimentally validated that the material size has a direct effect on its mechanical properties such as Young's modulus and flexural rigidity. He and Lilley [4,5] studied the surface effect on the elastic behaviour and the resonant frequency of bending for nanowires at different boundary conditions. Wong et al. [6] have experimentally measured the Young's modulus for silicon carbide nanorods while it was dynamically measured by Poncharal et al. [7]. Cuenot et al. [8] introduced surface stress to study the bending behaviour of nanowires. Jing et al. [3] measured the elastic properties of silver nanowires of different diameters. They found that Young's modulus decreases with increase in wire diameter, and they attributed that to the surface effect.

Classical continuum models do not take into account the effects of surface stresses and thus fail to present accurate models for such cases [2]. To account for surface energy effects, Gurtin and Murdoch [9] developed a surface elasticity theory for isotropic materials. In their model, the surface layer of a solid is treated as a membrane perfectly bonded to the material bulk. Lu et al. [10] modified the Gurtin-Murdoch model to develop a theory for modelling thin plates including surface effects. Surface energy effects on nanostructures have been studied by many researchers over the past decade. Bending properties of nanowires have been studied by Yun and Park [11] and Zhan et al. [12]. Liu and Rajapakse [13] presented closed-form solutions of static and free vibrating nanobeams under different boundary conditions considering surface stresses. Gheshlaghi and Hasheminejad [14] found exact solutions of the natural frequency of simply-supported nanobeams considering surface energy. Further, they used a dissipative surface stress model to study the effect size on natural frequencies of vibrating nanowires using Euler-Bernouli beam model [15] and Timoshenko beam model [16].

Since carbon nanotubes have significant waviness and curvature along the nanotubes length [17], it necessitates the consideration of curvature in the analysis of nano structures. Moreover, nanostructures can be exposed to different environmental and loading conditions, thus it is important to consider the effects of external thermal loads that may arise in such circumstances. In particular,

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the static stability of nanowires under thermal and mechanical loads is an important consideration since the wires undergo qualitatively large deformations once they undergo the pitch-fork bifurcation known commonly as buckling. Wang and Feng [18] studied the buckling of nanowires under uniaxial compression taking into account the effect of surface energy and residual surface tension. Wang and Yang [19] studied the effect of residual surface stress and surface elasticity on the post buckling state of nanowires under larger deflections using the shooting method.

Considering nonlocal elasticity, Mahmoud et al. [2] presented a static analysis of nanobeams including surface effects using the finite element method. Mohammadi et al. [17] studied the static instability of a curved nonlocal nanobeam on elastic foundation. Thongyothee and Chucheepsakul [20] investigated the post buckling of nanorods subjected to an end concentrated load, accounting for surface energy and nonlocal elasticity. They found that surface stress significantly increases structural stiffness and thus results in resisting post buckling load and end displacement. Lee and Chang [21] studied buckling of a cantilever nanowire with varying diameter considering surface effects and employing nonlocal elasticity. They found that the influence of surface effects on the critical buckling load is significant. Tounsi et al. [22,23] studied the thermal buckling of straight nanobeams where they employed a high-order beam theory using nonlocal elasticity. Further, using a nonlocal Timoshenko beam model, Semmah et al. [24] found that the critical buckling temperature is dependent on the chirality of zigzag carbon nanotubes.

To the knowledge of the authors, buckling analysis of curved nanowires under thermal loading and considering surfaces forces has not been addressed in literature. This work presents an effort towards investigating such conditions. In the present work, a model is developed to study the static buckling behavior of curved nanobeams under thermal loads, taking into account the surface effects. The beam is modelled as an Euler-Bernoulli beam with curvature, incorporating the surface constitutive relations of Gurtin and Murdoch. The mathematical model is presented in Section 2. Section 3 shows the results and parametric studies. Concluding remarks are then given in Section 4.

2. Model

Based on kinematic assumption of Euler-Bernoulli beam including nonlinear von Kármán strain (midplane stretching) and thermal strain, the axial strain of curved wire can be described by.

$$\varepsilon_{xx} = \frac{\partial u}{\partial x} + \frac{1}{2}\left(\frac{\partial w}{\partial x}\right)^2 + \frac{\partial w}{\partial x}\frac{\partial w_0}{\partial x} - \alpha_{th}\Delta T - z\frac{\partial^2 w}{\partial x^2} = \varepsilon_0 + zk_x \tag{1}$$

where u,w and w_0 are the axial displacement, transverse displacement, and initial rise of a generic point along the beam axis relative to the mid-plane. α_{th} and ΔT are, respectively, the thermal expansion coefficient of the nanowire and temperature difference between the wire and environment. The parameters ε_0 and k_x are the longitudinal and bending strains, respectively, which are described by

$$\varepsilon_0 = \frac{\partial u}{\partial x} + \frac{1}{2}\left(\frac{\partial w}{\partial x}\right)^2 + \frac{\partial w}{\partial x}\frac{\partial w_0}{\partial x} - \alpha_{th}\Delta T \tag{2.a}$$

$$k_x = -\frac{\partial^2 w}{\partial x^2} \tag{2.b}$$

The force resultant N and bending moment resultant M due to normal stress σ_{xx} can be described as.

$$N = \int_A \sigma_{xx}\mathrm{d}A = EA\varepsilon_0 \tag{3.a}$$

$$M = \int_A z\sigma_{xx}\mathrm{d}A = EIk_x \tag{3.b}$$

where I is the second area moment,A is the cross sectional area, and E is Young's modulus. Using the principle of virtual displacement, we obtain

$$0 = \int_0^L \left[(N\delta\varepsilon_0 + M\delta k_x) - \left(q\delta w + f\delta u + \overline{P}\frac{\partial w}{\partial x}\frac{\partial \delta w}{\partial x}\right)\right]\mathrm{d}x \tag{4}$$

where q and f are transverse and axial distributed forces (measured per unit length), and $\overline{P}$ is an applied axial compressive force at the boundaries. Substituting Eq. (3) into Eq. (4), the following equilibrium equations can be derived:

$$\delta u: \frac{\partial N}{\partial x} + f = 0 \tag{5.a}$$

$$\delta w: \frac{\partial}{\partial x}\left(N\frac{\partial w}{\partial x}\right) + \frac{\partial^2 M}{\partial x^2} + q - \overline{P} = 0 \tag{5.b}$$

According to Gurtin-Murdoch model, the constitutive relations of the surface can be expressed as

$$\sigma_{xx}^s = \tau_0 - \frac{\tau_0}{2}\left(\frac{\partial w}{\partial x}\right)^2 + (2\mu_0 + \lambda_0)\varepsilon_{xx} \quad \text{at } z = \pm\frac{h}{2} \tag{6.a}$$

$$\sigma_{xz}^s = \tau_0\frac{\partial w}{\partial x} \quad \text{at } z = \pm\frac{h}{2} \tag{6.b}$$

where τ_0 is the residual surface stress under no-load conditions, h is the thickness, andμ_0 and λ_0 are surface Lamé's constants, which can be determined from atomistic calculations. According to Euler beam theory, the stress componentσ_{zz} is small and thus neglected. However, σ_{zz} must be considered to satisfy the surface equilibrium which is assumed to vary linearly through the beam thickness [13]

$$\sigma_{zz} = \frac{2z\tau_0}{h}\frac{\partial^2 w}{\partial x^2} \tag{7}$$

Now, including the surface stress componentσ_{zz} of bulk stress of the nanobeam yields.

$$\sigma_{xx} = E\varepsilon_{xx} + \upsilon\sigma_{zz} \tag{8}$$

where E and υ are Young's modulus and Poisson's ratio, respectively.

Neglecting distributed axial and transverse forces q and f, the equilibrium equation of a clamped–clamped curved nanowire of length L including an axial force at the boundary $\overline{P}$, an axial thermal load, and surface stress effects can be described by [9,13]

$$\begin{aligned}&\left[EI - \frac{2\upsilon I\tau_0}{h} + (2\mu_0 + \lambda_0)I_s\right]\frac{\partial^4 w}{\partial x^4}\\ &+ \left[\overline{P} + EA\alpha_{th}\Delta T - \pi r\tau_0 - \frac{AE}{2L}\int_0^L\left(\left(\frac{\partial w}{\partial x}\right)^2 + 2\frac{\partial w}{\partial x}\frac{\partial w_0}{\partial x}\right)dx\right]\\ &\times\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w_0}{\partial x^2}\right) = 0\end{aligned} \tag{9.a}$$

subject to the boundary conditions