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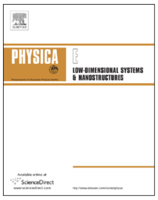

Mechanics of nanowire buckling on elastomeric substrates with consideration of surface stress effects

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HIGHLIGHTS

- The surface stress effects are considered in the analysis of the out-of-surface buckling behavior of a nanowire integrated on an elastomeric substrate.
- The surface effects can greatly influence the critical buckling strain and potential energy of the buckled nanowire.
- For nanowires with small cross section sizes and low bulk modulus, the buckling mode may be changed by tuning the surface properties.
- The range of the parameters where the out-of-surface buckling and in-surface buckling take place is explicitly determined with the energy criterion.

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ABSTRACT

In this paper, the surface stress effects are considered in the analysis of nanowire buckling on elastomeric substrates. Theoretical solutions of the buckling wavenumber, amplitude, and the critical strain for the out-of-surface buckling are derived firstly. After that, the influences of the surface properties, size, bulk modulus, and the shape of the cross section of the nanowire on the out-of-surface and in-surface buckling behavior are systematically discussed. Our study indicates that the buckling mode of the nanowire can be greatly influenced by the surface effects. For nanowires with small cross section sizes and low bulk modulus, the buckling mode may be varied by tuning the surface properties. Based on the energy criterion, we explicitly determine the range of the parameters where the two buckling modes take place.

1. Introduction

Buckling of thin stiff structures on elastomeric substrates has important applications in various fields, such as stretchable electronics [1–6], optical gratings [7], precision metrology [8–10], and flexible optoelectronics [11]. When integrated on compliant substrates in their buckled state, thin stiff structures can sustain large deformations in tension and compression, which provides an effective method to resolve the deformation incompatibility of stiff semiconductor materials and compliant substrates. Some researchers attempted to use nanostructures such as carbon nanotubes (CNTs) and silicon nanowires (SiNWs) to develop miniaturized flexible electronics [12,13]. Theoretical analysis of the buckling behavior of these nanostructures helps to guide the design of miniaturized devices. Xiao et al. studied the out-of-surface buckling behavior of CNTs on the PDMS substrate [14]. Analytical solutions of wavelength, amplitude, and critical buckling strain were derived. While most studies on structural buckling on compliant substrates assumed that the buckling takes place normal to the substrate, Ryu et al. reported for the first time that SiNWs on elastomeric substrates always buckle within the substrate surface, i.e., the in-surface buckling [15]. Based on this observation, Xiao et al. derived the theoretical solutions for the in-surface buckling of SiNWs and CNTs [16]. They compared the potential energy of the in-surface buckling and out-of-surface buckling and found that it is energetically favorable for the in-surface buckling to take place. It is noted that in all these studies, the linear elastic theory is applied to characterize the mechanical response of stiff structures. It is well known that for nanostructures, the influences of surface stress effects on their mechanical responses are non-negligible [17–20]. The surface elastic theories have been adopted to study the bending, vibration and buckling behavior of nanobeams and nanoplates [21–23]. These theories are still in their development stage. Li et al. [24] studied the out-of-surface wrinkling behavior of piezoelectric thin films on compliant substrates considering surface piezoelectricity. Recently, Wang et al. studied the influence of surface effects on the in-surface

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buckling behavior of nanowires on compliant substrates [25]. Their results indicate that the surface effects can greatly influence the out-of-surface and in-surface buckling behavior of nanostructures on the substrate medium.

This paper studies the out-of-surface buckling behavior of a nanowire integrated on a compliant substrate with consideration of the surface stress effects. In the analysis, the nanobeam theory based on the Gurtin–Murdoch model [26,27] and the Young–Laplace equation [17,28] is adopted. The theoretical solutions of the buckling wavenumber, amplitude, and the critical strain for the out-of-surface buckling are derived firstly. After that, the influences of the surface properties, size, bulk modulus, and the shape of the cross section of the nanowire on the out-of-surface and in-surface buckling behaviors are systematically discussed. Our results indicate that the buckling mode of the nanowire may be varied by tuning the surface properties, especially for nanowires with small size and low bulk modulus. We explicitly determine the range of the parameters where the two buckling modes take place with the energy criterion.

2. Formulations for the out-of-surface buckling

The integration process of a single nanowire on a compliant substrate is as follows [29,30]: a prepared nanowire is transferred to a prestrained PDMS substrate. After releasing the prestrain, the nanowire is buckled with a regular waveform. In this section, we assume that the nanowire buckles normal to the surface of the PDMS substrate. To the best knowledge of the authors, the out-of-surface buckling behavior of nanowires with consideration of the surface stress effects has not been studied in the open literature.

According to the nanobeam theory [17], the nanowire is divided into a surface layer and a core or bulk. Here we assume the cross section of the nanowire is rectangular. The Young's modulus of the bulk is E and the height and width of the cross section are denoted as h and b, respectively. The surface layer has a thickness t and elastic modulus E_1. The surface layer is assumed to be much smaller than the bulk, i.e., $t< <b,h$.

The surface stress of the nanowire is defined as Refs. [17,18],

$$\tau^s = E^s \varepsilon + \tau^0, \tag{1}$$

where $E^s = E_1 t$ is the surface elastic modulus, ε is the surface strain and τ^0 is the residual surface stress.

For the out-of-surface buckling as shown in Fig. 1, the effective bending stiffness $(EI)_1^*$ and effective tensile stiffness $(EA)^*$ of the nanowire can be expressed as

$$(EI)_1^* = \frac{1}{12}Ebh^3 + \frac{1}{2}E^s bh^2 + \frac{1}{6}E^s h^3, \tag{2}$$

$$(EA)^* = Ebh + 2E^s(b+h). \tag{3}$$

The residual surface stress results in a distributed vertical load $p(x)$ as shown in Fig. 1 along the longitudinal direction of the nanowire. For a rectangular nanowire, we have $p(x) = 2\tau^0 b\kappa_1(x)$, where $\kappa_1(x) = \partial^2 w/\partial x^2$ is the curvature of the buckled nanowire. The normal deflection w for the out-of-surface buckling can be described by a sinusoidal function $w = w_{\max}\cos k_1 x$, where $w_{\max}$ is the buckling amplitude, k_1 is the buckling wavenumber which is related to the wavelength λ_1 by $k_1 = 2\pi/\lambda_1$. The bending energy per unit length in the nanowire is

$$U_b = \frac{1}{\lambda_1}\int_0^{\lambda_1} \frac{1}{2}(EI)_1^*\left(\frac{d^2w}{dx^2}\right)^2 dx = \frac{(EI)_1^*}{4} w_{\max}^2 k_1^4. \tag{4}$$

The membrane strain ε_m in the nanowire can be expressed in terms of the normal deflection w and the axial displacement u by $\varepsilon_m = du/dx + (dw/dx)^2/2$. Since the Young's modulus of the nanowire ($\sim$140 GPa for SiNWs) is several orders of magnitude larger than that for the substrate ($\sim$2 MPa), the shear stress between the nanowire and the substrate is negligible, which results in a constant membrane force [14]. The axial displacement of the nanowire can be obtained as $u = k_1 w_{\max}^2 \sin(2k_1 x)/8 - \varepsilon_{pre} x$, where $-\varepsilon_{pre} = -(k_1^2 w_{\max}^2/4 - \varepsilon_m)$ is the compressive strain in the nanowire induced by the relaxation of the prestrain of the substrate. Therefore the membrane strain of the nanowire is $\varepsilon_m = k_1^2 w_{\max}^2/4 - \varepsilon_{pre}$, from which the axial deformation energy per unit length in the nanowire can be obtained as

$$U_m = \frac{1}{\lambda_1}\int_0^{\lambda_1} \frac{1}{2}(EA)^* \varepsilon_m^2 dx = \frac{1}{2}(EA)^*\left(\frac{1}{4}k_1^2 w_{\max}^2 - \varepsilon_{pre}\right)^2. \tag{5}$$

The potential energy of the distributed vertical load due to the residual surface stress per unit length is

$$U_r = -\frac{1}{\lambda_1}\int_0^{\lambda_1} \tau^0 b \frac{d^2 w}{dx^2} w dx = \frac{1}{2}\tau^0 b w_{\max}^2 k_1^2. \tag{6}$$

And we have the following equilibrium equation of the nanowire:

$$-(EI)_1^*\frac{\partial^4 w}{\partial x^4} + 2\tau^0 b\frac{\partial^2 w}{\partial x^2} + (EA)^*\varepsilon_m \frac{\partial^2 w}{\partial x^2} + T_1 = 0 \tag{7}$$

here T_1 is the vertical force imposed by the substrate and it takes a sinusoidal form $T_1 = -P_1 \cos k_1 x$, where $P_1 = -(EI)_1^* w_{\max} k_1^4 - [(EA)^*\varepsilon_m + 2\tau^0 b] w_{\max} k_1^2$.

The PDMS substrate is modeled as a semi-infinite solid and its surface effects can be neglected since the thickness of the substrate is several orders of magnitude larger than the buckling wavelength of the nanowire. Let E_s denote the elastic modulus of the substrate and υ_s is the Poisson's ratio. For PDMS substrate, υ_s can be approximated as 0.5 since it is nearly incompressible. The substrate surface is traction-free except for the region underneath the nanowire, which has the width $2R = b$, and is along x direction. The normal stress traction in this region is the average of the

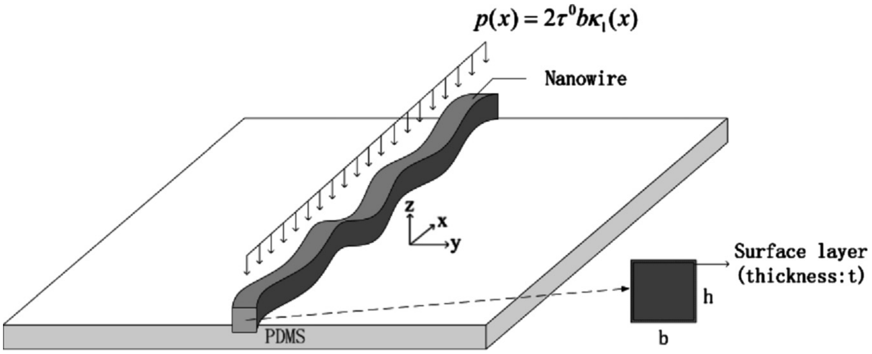

Fig. 1. The out-of-surface buckling of a rectangular nanowire on a PDMS substrate. The distributed load due to the residual surface stress is normal to the substrate.