MECHANICS OF NANOWIRE/NANOTUBE IN-SURFACE BUCKLING ON ELASTOMERIC SUBSTRATES

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Summary A continuum mechanics theory is established for the in-surface buckling of one-dimensional nanomaterials on compliant substrates. Simple analytical expressions are obtained for buckling wavelength, amplitude and critical buckling strain. For silicon nanowires, the measured buckling wavelength gives the Young's modulus to be 140 GPa, which agrees well with previous studies. It is shown that the energy for in-surface buckling is lower than that for out-of-surface buckling, and is therefore energetically favorable.

BACKGROUND AND EXPERIMENT

Buckling of thin layers or aligned arrays of stiff materials on elastomeric substrates has many important applications, such as stretchable electronics [1-11], precision metrology [12-14] and flexible optoelectronics [15]. These systems show normal buckling, i.e., the stiff thin layers buckle normal to the substrate surface. Their mechanics is well understood [16-24]. By contrast, Ryu et al. [25] recently reported for the first time that silicon nanowires (SiNWs) on elastomeric substrates buckle only within the substrate surface, i.e. in-surface buckling. Figure 1(a) summarizes the experimental process used in this case. SiNWs were first prepared on Si substrates using Au nanoclusters as catalysts in a vapor-liquid-solid (VLS) process. Each nanocluster served as a site that directs preferential addition of reactant to the end of a growing SiNW. Next, the randomly oriented SiNWs formed in this way were transferred, using shear force, to another silicon wafer substrate to form aligned arrays (Fig. 1(a), top frame) [26-28]. These arrays were then transferred to a prestrained PDMS substrate (uniaxial tensile along the lengths of the SiNWs) [29-32]. After releasing the prestrain, the resulting collection of buckled SiNWs (Fig. 1(a), bottom frame) was examined by atomic force microscope (AFM) and field-emission scanning electron microscope (FE-SEM) images. Figure 1 (b) shows some representative results.

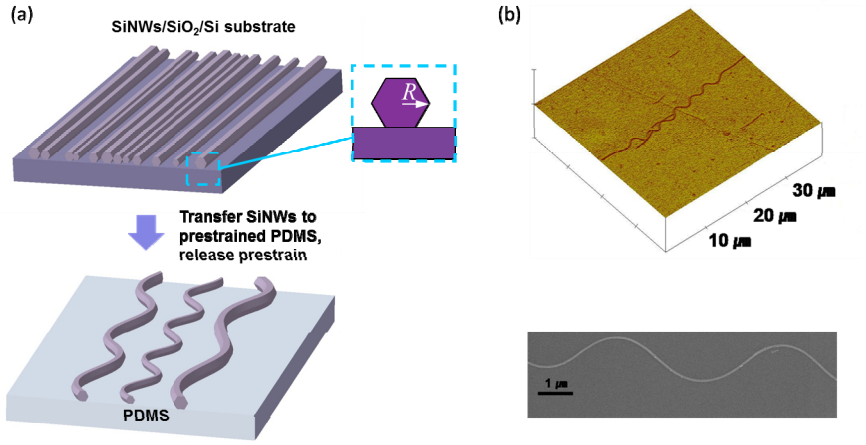

Figure 1. (a) Schematic diagram of the process to form laterally (in-surface) buckled, wavy SiNWs on PDMS substrates. (b) AFM (top) and FE-SEM (bottom) images of laterally buckled SiNWs on PDMS substrates.

BUCKLING MECHANICS OF ONE-DIMENSIONAL NANOMATERIALS ON COMPLIANT SUBSTRATE

Let EI and EA denote the bending and tension stiffness of a stiff beam on the surface of a compliant substrate, respectively. The lateral deflection v within the substrate surface of the buckled beam can be described by a sinusoidal form $v = v_{\max}\cos kx$, where the coordinate x is along the beam axis, $v_{\max}$ is the buckling amplitude, and the wave vector k is related to the wavelength λ by $k = 2\pi/\lambda$. The total energy of the system consists of the bending energy U_b and membrane energy U_m in the stiff beam, and strain energy U_S in the substrate, which is obtained as

$$\Pi_{tot} = \frac{EI}{4}v_{\max}^2 k^4 + \frac{EA}{2}\left(\frac{k^2 v_{\max}^2}{4} - \varepsilon_{pre}\right)^2 + \frac{1}{2}Pv_{\max} - \frac{P^2}{4\pi\bar{E}_S}\left(\frac{3-\nu_S}{1-\nu_S} - 2\gamma - 2\ln kw\right), \tag{1}$$

Minimization of Π_{tot} with respect to $v_{\max}$ and k gives the following equations,

$$\left(EI/\bar{E}_S\right)^{1/4} k = \left[2\pi\left(\frac{1}{1-\nu_S} - \gamma - \ln kw\right)\Big/\left(\frac{3-\nu_S}{1-\nu_S} - 2\gamma - 2\ln kw\right)^2\right]^{1/4}, \quad v_{\max} = \frac{2}{k}\sqrt{\varepsilon_{pre} - \varepsilon_c}, \tag{2}$$

where $\varepsilon_c = \left\{ EIk^4 + \pi \bar{E}_S \left[(3-\nu_S)(1-\nu_S)^{-1} - 2\gamma - 2\ln kw \right]^{-1} \right\} \Big/ \left(EAk^2 \right)$ is the critical buckling strain of a stiff beam on a compliant substrate. The right hand side of first equation in Eq. (2) is essentially a constant because both logarithmic and one-fourth power functions change very slowly with *kw*. For a nearly incompressible substrate such as PDMS, $\nu_S \approx 1/2$, this constant is approximately 5/7 such that the wave vector *k* and wavelength λ are given as

$$k = \frac{5}{7}\left(\frac{\bar{E}_S}{EI} \right)^{1/4}, \qquad \lambda = \frac{14\pi}{5}\left(\frac{EI}{\bar{E}_S} \right)^{1/4}. \tag{3}$$

For SiNWs, the cross section is hexagon of radius R, as shown in Fig. 1(a). Its moment of inertia and cross sectional area are $I_{SiNW} = \left(5\sqrt{3}/16\right)R^4$ and $A_{SiNW} = \left(3\sqrt{3}/2\right)R^2$, respectively. It has one side in contact with the substrate surface, thus the width of the contact region $2w_{SiNW} = R$. The wavelength and amplitude are obtained as

$$\lambda_{SiNW} = \frac{12\pi R}{5}\left(\frac{E_{SiNW}}{\bar{E}_S} \right)^{1/4}, \quad \left(\nu_{\max} \right)_{SiNW} = \frac{\lambda_{SiNW}}{\pi}\sqrt{\varepsilon_{pre} - \left(\varepsilon_c \right)_{SiNW}}. \tag{4}$$

The buckling wavelength and amplitude are compared with experiment in Figure 2, showing good agreement. For PDMS Young's modulus $E_S = 2\ MPa$ and Poisson's ratio $\nu_S = 0.5$, Fig. 2(a) yields the Young's modulus of SiNW $E_{SiNW} = 140\ GPa$, which agrees well with prior values reported for SiNW.

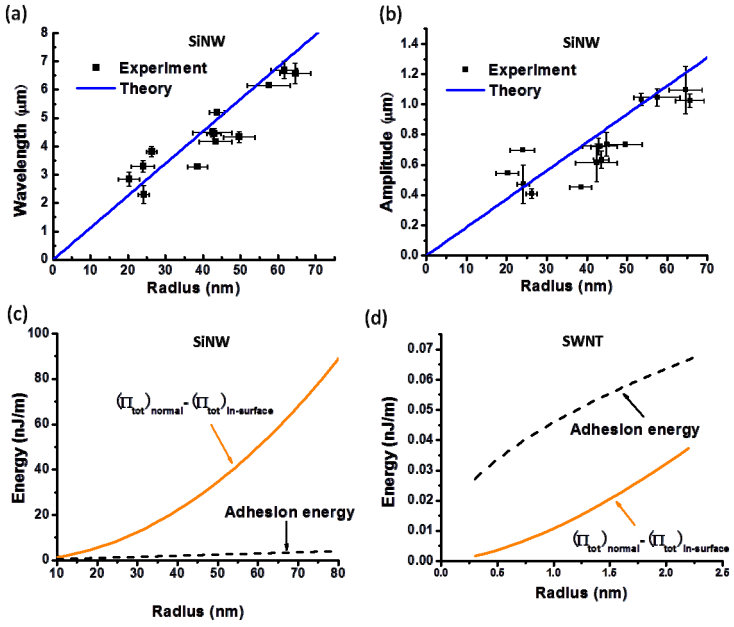

Figure 2. (a) In-surface buckling wavelength versus SiNW radius. (b) In-surface buckling amplitude versus SiNW radius. (c) Energy difference between normal and in-surface buckling, and the adhesion energy between SiNWs and PDMS, versus SiNW radius. (d) Energy difference between normal and in-surface buckling, and the adhesion energy between SWNTs and PDMS, versus SWNT radius.

Rather than normal buckling, SiNWs buckle within the surface of PDMS in the experiments because the in-surface buckling mode gives lower potential energy. For $\varepsilon_{pre} = 27\%$ as in experiments, Fig. 2c shows that the potential energy for normal buckling [20] is larger than that in Eq. (1) for in-surface buckling, and their difference increases rapidly with the SiNW radius. This explains the experimentally observed in-surface buckling of SiNWs. For comparison, Fig. 2c also shows the adhesion energy between SiNWs and PDMS. The energy difference between normal and in-surface buckling is much larger than the adhesion energy, particularly at relatively large radius. The above analysis is also applied to single-walled carbon nanotubes (SWNTs), multi-walled carbon nanotubes (MWNTs) and carbon nanotube bundles. For SWNTs, the normal buckling also has a higher energy than in-surface buckling. However, as shown in Fig. 2d their difference is much smaller than the adhesion energy between SWNTs and PDMS. Furthermore, the surface roughness of PDMS is comparable to or even larger than the SWNT radius (~ 1 nm), thereby giving rise to the possibility that this roughness can prevent the in-surface buckling mode [25].

CONCLUSIONS

A continuum mechanics theory is established for the in-surface buckling of one-dimensional nanomaterials on compliant substrates. Simple analytical expressions are obtained for buckling wavelength, amplitude and critical buckling strain, which show good agreement with experiment. It is shown that the energy for in-surface buckling is lower than that for out-of-surface buckling, and is therefore energetically favorable.

References

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