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Analysis of uniaxial compression of vertically aligned carbon nanotubes

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ABSTRACT

We carry out axisymmetric, finite deformation finite element analyses of the uniaxial compression of cylindrical bundles of vertically aligned carbon nanotubes (VACNTs) firmly attached to a Si substrate. A compressible elastic–viscoplastic constitutive relation with a piecewise, linear hardening–softening–hardening flow strength is used to model the material. Calculations are performed for VACNTs both with uniform properties and with axially graded properties. We show that, with uniform properties, sequential buckling initiates at the substrate and propagates away from it, in agreement with previous experimental findings. We investigate the dependence of the magnitude and wavelength of the buckles on characteristics of the function defining the flow strength. When a property gradient giving a more compliant response at the end opposite to the substrate is specified, we find that sequential buckling initiates at that end and propagates toward the substrate. Results of the analyses are compared with the experimental observations and capture many of the experimentally obtained stress–strain and morphological features. The proposed model serves as a promising foundation for capturing the underlying energy absorption mechanisms in these systems. Comparison of the model predictions with the experimental results also suggests directions for model improvement.

1. Introduction

Vertically aligned carbon nanotubes (VACNTs), referred to within the literature as carbon nanotube (CNT) forests, turfs, brushes, and mats, have shown promising mechanical properties for use in a variety of applications, for example, viscoelastic energy absorption (Cao et al., 2005; Gogotsi, 2010; Misra et al., 2009; Pathak et al., 2009; Xu et al., 2010; Zhang et al., 2010), compliant thermal interfaces (Cola et al., 2009; McCarter et al., 2006; Zbib et al., 2008), and biomimetic dry adhesives (Boesel et al., 2010). A fundamental understanding of their mechanical behavior is of paramount importance as it provides the basis for design in these applications as well as for in-use lifetime analysis in the various VACNT technologies in which mechanical properties may be of secondary importance. Several groups have published studies of the mechanical properties of VACNTs measured through nanoindentation (McCarter et al., 2006; Mesarovic et al., 2007; Pathak et al., 2009; Qiu et al., 2011), uniaxial compression (Cao et al., 2005; Hutchens et al., 2010; Raney et al., in press; Suhr et al., 2007; Tong et al., 2008; Zbib et al., 2008), and impact testing (Daraio et al., 2006; Misra et al., 2009). Variations

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in observed behavior and quantitative results in these publications illustrate that the wide variety of growth conditions that can, in turn, result in significant dissimilarities in the mechanical properties, including deformation morphology, the amount of post-deformation recovery, and the elastic modulus. In particular, some VACNTs display high recoverability after significant strain (Cao et al., 2005) while others have been observed to deform permanently (Hutchens et al., 2010; Yaglioglu, 2007; Zbib et al., 2008). This paper aims to provide insight into the largely irrecoverable deformation observed after uniaxial compression of the VACNT bundles observed by Hutchens et al. (2010) and others (Zbib et al., 2008; Zhang et al., 2010) as opposed to highly recoverable and/or viscoelastic behavior (Cao et al., 2005; Gogotsi, 2010; Pathak et al., 2009; Xu et al., 2010; Zhang et al., 2010), though many similarities exist between the two, particularly the localization of deformation via buckling under uniaxial compression (Cao et al., 2005; Hutchens et al., 2010; Yaglioglu, 2007; Raney et al., in press; Zbib et al., 2008). As illustrated in Fig. 1, this rich behavior is characterized by the accommodation of strain through the creation of a series of vertically localized folds or buckles, which form sequentially starting from the base (where CNTs grow from the substrate) and proceed toward the top (Cao et al., 2005; Hutchens et al., 2010; Yaglioglu, 2007; Zbib et al., 2008) (see Fig. 1c), and the initiation of buckles followed by their lateral propagation as revealed through *in situ* deformation of micron-sized cylindrical bundles, or pillars by Hutchens et al. (2010) (see Fig. 1b). Fig. 1a shows the overall foam-like stress–strain response gathered during testing. The response consists of elastic, plateau, and densification regimes typical of these materials (Cao et al., 2005). The plateau possesses a small hardening slope. Here, we plot nominal stress, $\sigma_n = P/A_0$, versus nominal strain, $\varepsilon_n = \Delta H/H$, where P is the applied load, A_0 is the initial area of the top of the pillar, H is the initial pillar height, and ΔH is the displacement of the top. We find that immediately following the elastic loading the load drops sharply before reaching the sloped plateau characterized by periodic softening events shown to correspond to the appearance and evolution of individual buckling events (Hutchens et al., 2010). This correspondence is illustrated in the image series in Fig. 1b for strains denoted by the blue circles in Fig. 1a.

While there are several experimental studies showing this highly localized commencement of structural collapse, models describing the mechanical response of VACNTs are few and past efforts have focused on capturing only the one-dimensional stress–strain or load–displacement response. For example, the load–displacement response has been modeled energetically as well as in a standard linear solid framework and compared with nanoindentation testing results

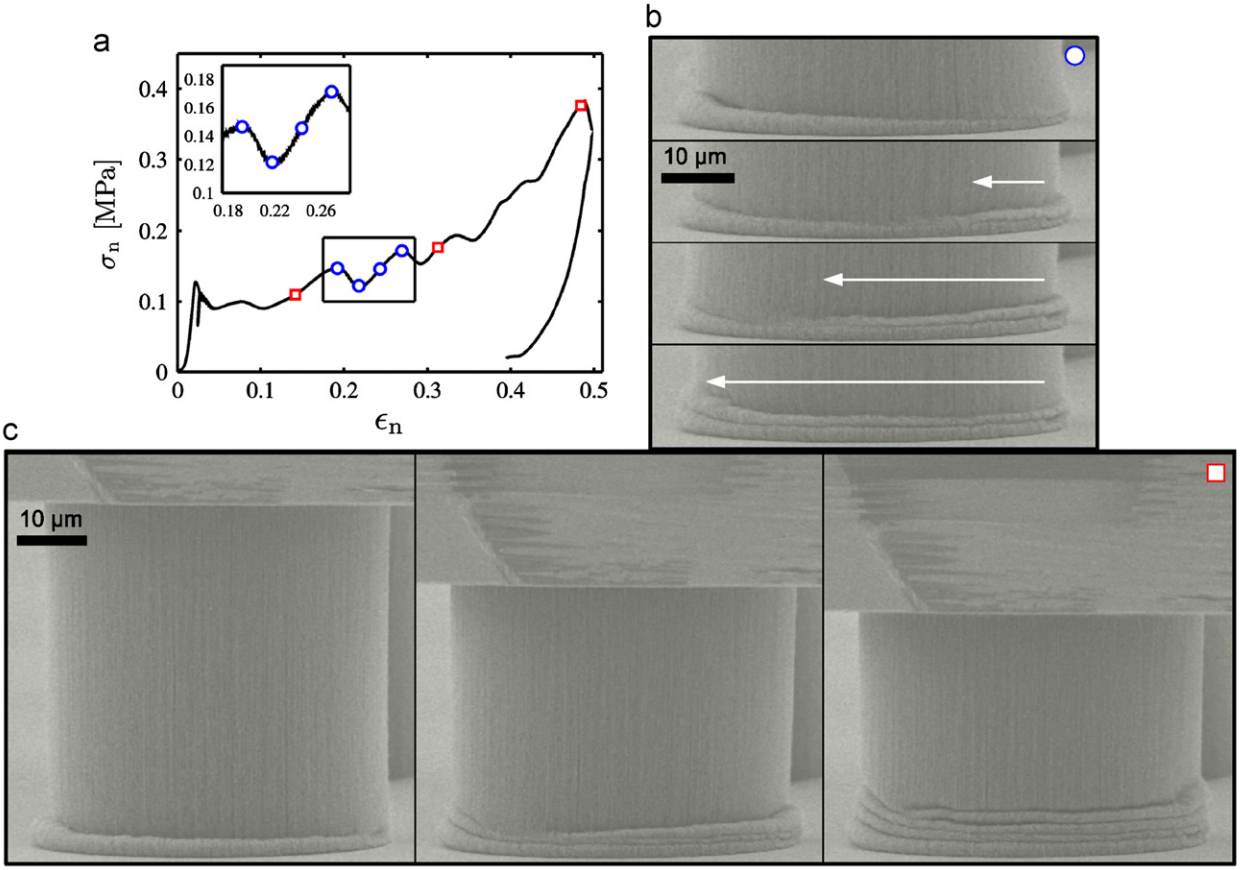

Fig. 1. *In situ* mechanical compression results using methods presented in Hutchens et al. (2010). (a) Nominal stress–strain response. Blue circles and red squares denote the strains at which the images in (b) and (c) were taken. (b) Illustrates buckle initiation and evolution. (c) Illustrates bottom-to-top sequential buckling. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)