

Buckling Instabilities in Multi-walled Carbon Nanotubes

I. Background and Scope: Since carbon nanotubes are slender, thin-walled structures, they are highly susceptible to buckling when loaded in axial compression, which results in a sudden drop in the load they can support, often leading to fracture. Although researchers have been successful in manipulating individual nanotubes to induce tension, bending and vibration, uniaxial compression experiments have been hindered by the difficulty of achieving properly aligned axial loading on such small structures. It is important to be able to predict the onset of buckling for many nanotube applications such as scanning probe tips and nanotube fiber–polymer composites. Here, we developed a new experimental technique for uniaxial compression of nanotubes in order to enable systematic studies of the buckling behavior of multi-walled carbon nanotubes and for development of refined continuum models of nanotube mechanics.

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III. Significant Results

Carbon Nanotube Samples: Highly regular arrays of uniform nanotubes embedded in an alumina matrix were fabricated through a CVD process. The nanotubes in this study were spaced 100 nm apart and had 50 nm outer diameter and 40 nm inner diameter. The wall thickness of 5 nm corresponds to approximately 15 walls. A forest of vertically standing nanotubes is then obtained by etching the alumina matrix by any desired depth, as shown in Fig. 1. In our experiments, two sets of samples were made, on which the exposed heights of the nanotubes were 100 nm and 50 nm, respectively. These relatively short lengths ensure that compressive loading will cause shell buckling in the nanotubes, rather than the column buckling.

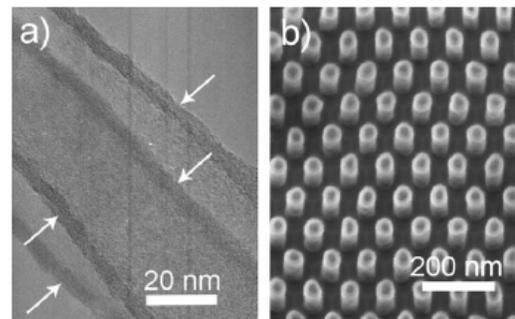


Figure 1. (a) TEM image of multi-walled nanotubes showing the wall thickness. (b) SEM image of an ordered array of nanotubes in alumina matrix.

Shell-buckling experiments on individual nanotubes with nanoindentation:

An experimental technique is developed for precise uniaxial compression of an individual nanotube in the array shown in Fig. 1b. The experimental arrangement is shown schematically in Figure 2, along with a representative load-displacement curve. The specimen is imaged before and after the indentation in order to ascertain the accuracy of locating and compressive the targeted nanotube. The loading portion consists of three stages: an initial linear (approximately) increase, followed by a sudden drop in the slope and the curve becoming flat, and a third stage comprising an increasing load. The sudden decrease in the slope is the signature of shell buckling, which indicates the collapse process illustrated in Fig. 2b. The critical buckling load has been consistently measured to be between 2 and 2.5 μN from multiple experiments. After buckling, neighboring nanotubes come into contact with the indenter tip, which results in an increase in load in the third stage. The salient feature of these experiments is the precise control of the specimen geometry and loading configuration so that we can obtain readily interpretable data that can serve as a basis for developing continuum models.

General Shell Buckling of Shear-Coupled Multiwalled Carbon Nanotubes:

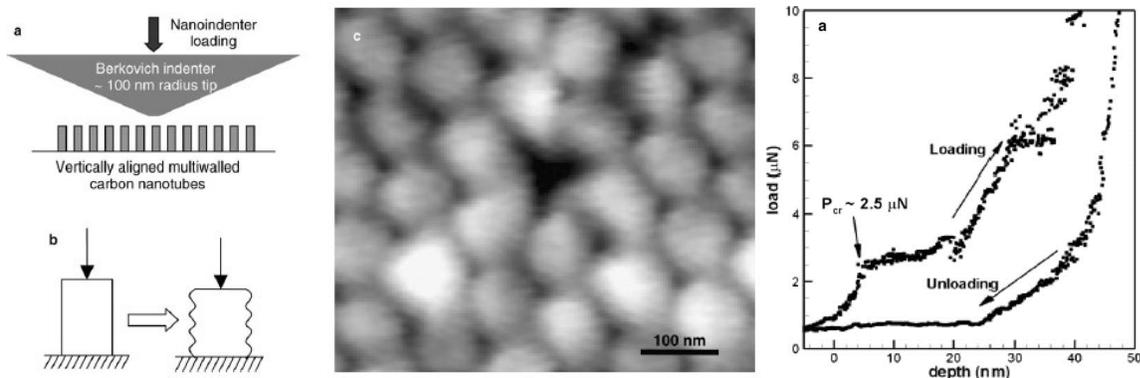


Figure 2. (a) Schematic illustration of the experiment in which a Berkovich indenter with 100 nm tip radius vertically compresses a multi-walled carbon nanotube. (b) Schematic illustration of shell buckling in nanotubes, which results in a load collapse and severe distortion of the nanotube walls. (c) An in situ scanning image of the sample surface obtained immediately after compressing a nanotube, by using the indenter tip as the scanning probe. The buckled nanotube is shorter than the neighboring nanotubes, resulting in a dark spot in the topographic image.

It turns out that the classical shell buckling models under predict the shell buckling load by nearly 50%. Through Raman spectroscopy, we have identified the source of the discrepancy to the presence of imperfections in the nanotubes in the form of sp^3 bonds between neighboring walls, which increase the shearing resistance between the walls. Based on these observations, we developed a general shell buckling model for shear-coupled multi-walled carbon nanotubes. The analysis results in a corrective term for critical buckling strain, which is proportional to the “shearing modulus” transverse to the walls. The model accurately describes the experimental results and the observed buckling mode. We have extended the study by carrying out molecular dynamics calculations of the multi-walled carbon nanotubes with sp^3 impurities and verified that the shear coupled shell buckling theory captures the MD results over the entire range investigated (Fig 3.). We have also shown that the shear coupled shell model accurately captures the predictions of a transversely isotropic shell theory as well.

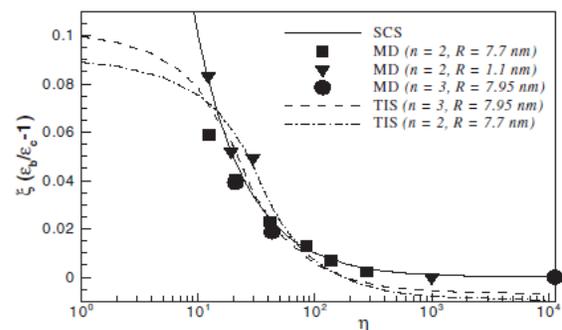


Figure 3. Normalized buckling strain ϵ_b of MWCNTs, vs. the nondimensional interwall shear parameter η predicted by MD simulation, and SCS (shear coupled shell theory) and TIS (transversely isotropic shell theory) models.

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V. Publications:

1. Z. Xia, P.R. Guduru and W. Curtin. Enhancing Mechanical Properties of Multi-Wall Carbon Nanotubes via sp^3 Inter-wall Bridging. *Physical Review Letters* 98: Art. No. 245501, 2007.
2. P.R. Guduru and Z. Xia. Experiments and Analysis of Buckling in Imperfect Multiwalled Carbon Nanotubes (Invited contribution to a special volume on novel testing techniques at nanoscale). *Experimental Mechanics* 47: 153-161, 2007.
3. J.F. Waters, P.R. Guduru and J.M. Xu. Nanotube Mechanics – Recent Progress in Shell Buckling Mechanics and Quantum Electromechanical Coupling. *Composites Science and Technology*. 66: 1141-1150, 2006.
4. J.F. Waters, P.R. Guduru, T. Hanlon, M. Jouzi, J.M. Xu and S. Suresh. Shell Buckling of Individual Multi-walled Carbon Nanotubes Using Nanoindentation. *Applied Physics Letters* 87: 103109, 2005.
5. J.F. Waters, L. Riester, M. Jouzi, P.R. Guduru and J.M. Xu. “Buckling instabilities in multiwalled carbon nanotubes under uniaxial compression.” *Applied Physics Letters*, 85: 1787-1789, 2004.