Radial Deformability of Carbon and Boron Nitride Nanotubes

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Summary The radial deformability of individual single- and multi-walled carbon and boron nitride nanotubes is characterized by using atomic force microscopy. Our results show that the effective radial moduli of both types of tubes increase with the number of tube layers and decrease with the increase of the tube outer diameter. Our study reveals that boron nitride nanotubes have relatively lower effective radial moduli than comparable carbon nanotubes.

INTRODUCTION

Carbon and boron nitride nanotubes (CNTs and BNNTs) are two similar types of one-dimensional nanostructures, composed of repeated covalent C-C and partially ionic B-N bonding networks, respectively. Both types of tubes possess extraordinary mechanical properties, thermal conductivity and chemical stability, while their electrical properties are distinctly different. Unlike the semi-conductive or metallic properties of CNTs, BNNTs possess a large band-gap (~5-6 eV) and thus are excellent electrical insulators. CNTs hold tremendous potentials for a variety of applications, such as composites, electronics, sensors and biomedicines, while BNNTs are promising for applications of composites, protective shields/capsules, and electrical insulators. The radial deformability of CNTs and BNNTs is an important issue for a complete understanding of their structural and material properties and many of their applications. For instance, radial rigidity of nanotubes is relevant to their structural configurations in a bundle or rope, or when they are in contact with other materials surfaces. The radial deformation of nanotubes is also found to influence their electronic band structures. In this paper, we present and discuss the experimental characterization of the radial mechanical properties of single- and multi-walled CNTs and BNNTs using atomic force microscopy (AFM).

EXPERIMENTS AND METHODS

AFM Measurements

The radial deformability of both CNTs and BNNTs was characterized inside a high-resolution atomic force microscope (XE-70, Park Systems) operating in contact-mode using silicon AFM cantilevers (model CSG 11, NT-MDT) with nominal spring constants of 0.01-0.08 N/m. The employed CNTs and BNNTs were synthesized using chemical vapor deposition (CVD) and pressurized vapor/condenser (PVC) [1] methods, respectively. As illustrated by Figure 1(a), the AFM tip was controlled to scan an individual nanotube on a silicon substrate in contact mode at a specified compressive load with the scanning direction perpendicular to the tube axis. The applied compressive load (P) is calculated as the product of the calibrated spring constant of the employed AFM probe and its vertical deflection that was measured with a sub-angstrom resolution using laser-reflection schemes.

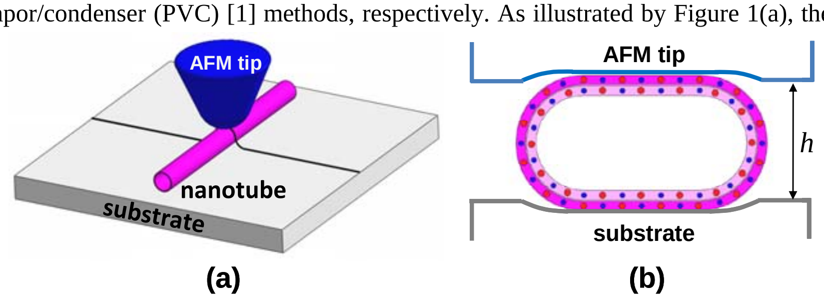

Figure 1 (a) Schematic of the AFM-based compression testing scheme on the radial deformation of an individual BNNT on a flat substrate. (b) Schematic of the deformations of a double-walled nanotube, an AFM tip and a substrate along the nanotube's transverse direction under a compressive load.

Contact Mechanics Models

Our AFM nanomechanical measurements on the radial deformation of both CNTs and BNNTs were interpreted using Hertzian contact mechanics models. The contacts between the AFM tip, the nanotube and the substrate are simplified as an elastic nanoindentation system consisting of a spherical tip, a cylindrical tube and a flat substrate. The effective radial modulus of each tested nanotube is obtained by fitting the measured compressive load (P) *versus* the nanotube cross-section height (h) curve using the following Hertzian model [2],

$$h = 2h_0 - P^{2/3}\left(\left(k_1\sqrt{h_0}\right)^{-2/3} - \left(k_2\sqrt{1/h_0 + 1/R_{tip}}\right)^{-2/3} + \left(k_3\sqrt{R_{tip}}\right)^{-2/3}\right), \quad (1)$$

$$k_1 = 4/3\left[\left(1-\nu_{nt}^2\right)/E_{nt}^{rad} + \left(1-\nu_{sub}^2\right)/E_{sub}\right]^{-1}, \quad k_2 = 4/3\left[\left(1-\nu_{tip}^2\right)/E_{tip}\right]^{-1}, \quad k_3 = 4/3\left[\left(1-\nu_{tip}^2\right)/E_{tip} + \left(1-\nu_{sub}^2\right)/E_{sub}\right]^{-1},$$

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where E and ν represent the elastic modulus (effective radial elastic modulus for nanotubes) and Poisson's ratio, respectively, for materials of nanotubes (subscript-*nt*), AFM tips (*tip*) and substrates (*sub*). h_0 represents the original cross-section height of the tested nanotube on the substrate and is estimated through power-function fitting and interpolation of the measured height h to zero load. R_{tip} is the radius of curvature of the employed AFM tips and is estimated to be ~25 nm. The first term inside the bracket on the right side of Eqn (1) represents the deformations of both the nanotube and the substrate due to the nanoindentation of the nanotube-substrate system. The second term represents the deformation of the AFM tip due to its contact with the nanotube (the nanotube is considered as a rigid body here to avoid double-counting its deformation). The last term represents the deformation of the substrate due to the nanoindentation of the AFM tip.

RESULTS AND DISUCSSION

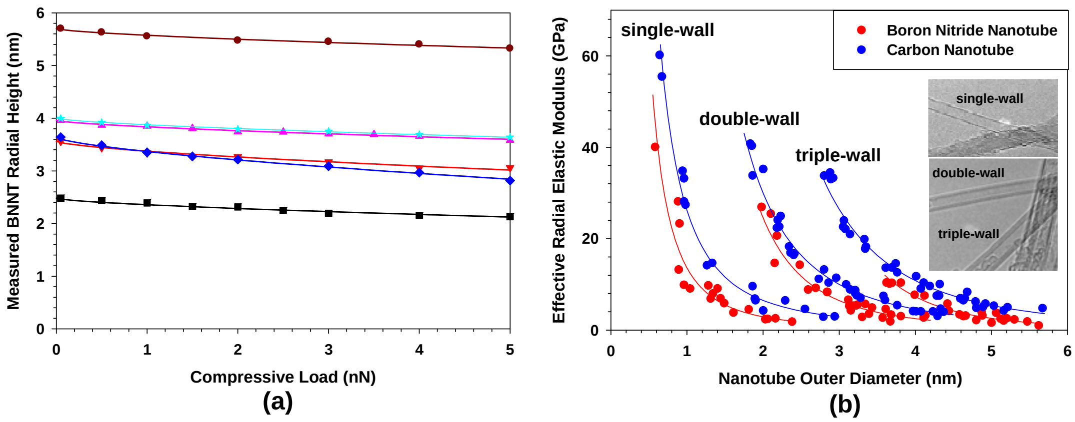

Figure 2 (a) The respective radial deformation profiles measured on six different BNNTs. The solid lines are the respective fitting curves of the experimental data (dots) based on the Hertzian model. (b) The dependences of the effective radial modulus on the nanotube outer diameter and the number of tube layers for single to triple-walled CNTs and BNNTs. The inset images are representative high resolution transmission electron microscopy (HRTEM) images of single to triple-walled BNNTs.

The effective radius moduli of individual nanotubes are calculated based on AFM compression measurements with the compressive load of up to 5 nN, under which the radial deformation of the nanotube was measured to be purely elastic. The number of tube layers in a nanotube was determined using minimal height approaches, i.e. measuring the cross-section height of the nanotube under a large compressive load (e.g. 50 nN). Figure 2(a) shows the radial deformation measurements on six different BNNTs with original tube heights (h_0) from 2.48 to 5.70 nm and their respective fitting curves based on the Hertzian contact model given by Eqn (1). Figure 2(b) shows the dependences of the effective radial modulus on the nanotube outer diameter and the number of tube layers for both CNTs and BNNTs of single to triple-wall [3, 4]. Our results consistently show that the effective radial moduli of both types of tubes increase with the number of tube layers and decrease with the increase of the tube outer diameter. Both single- and multi-walled BNNTs are found to have relatively lower effective radial moduli than their CNT counterparts. Our results suggest that BNNTs will more readily undertake hexagonal cross-section conformations in bundles than comparable CNTs, leading to more tightly bound yarns or ropes. In addition, BNNTs will be energetically more favourable for large-angle bending and buckling, an advantage over CNTs as reinforcing additives in polymeric and ceramic nanocomposites.

CONCLUSIONS

In this paper, we present an AFM study on the radial mechanical properties of single- and multi-walled CNTs and BNNTs. Our results reveal that the effective radial moduli of both types of tubes increase with the number of tube layers and decrease with the increase of the tube outer diameter, and BNNTs have relatively lower effective radial moduli than comparable CNTs. Our findings of the radial deformability of both CNTs and BNNTs are useful to the pursuit of tuning their electrical properties (e.g. band-gap) through mechanical deformations. Our work contributes directly to a complete understanding of the fundamental structural and mechanical properties of CNTs and BNNTs and the pursuits of their novel structural and electronics applications.

References

[1] Smith M.W., Jordan K.C., Park C., Kim J.W., Lillehei P.T., Crooks R. and Harrison J.S., *Nanotechnology*, 20: 505604, 2009.
[2] Yang Y.H. and Li W. Z., *Appl. Phys. Letts*., 98: 041901, 2011.
[3] Zheng M., Chen X.-M., Bae I.-T., Ke C.-H., Park C., Smith M.W., Jordan K., *Small, in press*, 2011. DOI: 10.1002/smll.201100946.
[4] Zheng M., Ke C.-H., Bae I.-T., Park C., Smith M.W., Jordan K., submitted to *Nanotechnology*, 2011.