On the Mechanical Behavior of Boron Nitride Nanotubes

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Boron nitride (BN) nanotubes have structural and mechanical properties similar to carbon nanotubes and are known to be the strongest insulators. Great interest has been focused on understanding the mechanical properties of BN nanotubes as a function of their structural and physical properties. Yet, the published data have not been reviewed and systematically compared. In this paper, we critically review the mechanical properties of BN nanotubes from both experimental and simulation perspectives. The experimental reports include thermal vibrations, electric induced resonance method, and in situ force measurements inside transmission electron microscopy. The modeling and simulation efforts encompass tight bonding methods and molecular dynamics. Replacing the covalent sp^2 bond (C–C) by ionic bond (B–N) results in differences in the mechanical properties of BN nanotubes in comparison to carbon nanotubes. The experimental and computational simulations indicate that BN nanotubes are highly flexible. High necking angles in BN nanotubes are assumed to be correlated with unfavorable bonding in B–B and N–N atoms. [DOI: 10.1115/1.4001117]

Keywords: boron nitride nanotubes, mechanical properties, modeling and simulation, Young's modulus

1 Introduction

The discovery of various types of nanotubes has provided fertile ground for both experimental and complementary theoretical studies. A boron nitride (BN) nanotube has structural analog similar to a carbon nanotube in nature, where alternating B and N atoms entirely substitute for C atoms in a graphiticlike sheet, as shown in Fig. 1.

Different methods of BN nanotube synthesis are available such as arc discharge [1], laser ablation [2], and substitution reaction [3]. But the most efficient method which is capable of synthesizing a reasonable amount of BN nanotubes is by chemical vapor deposition (CVD) [4]. For pure carbon nanotubes, theoretical calculations predict that mechanical properties depend on the radius and chirality of the nanotubes [5]. However, some degree of difference in the mechanical properties due to change in the electronic structure of BN nanotubes is expected. Replacing the strong covalent sp^2 bond between carbon atoms by B–N ionic bond is the main difference between BN and carbon nanotubes. BN nanotubes show a preference for zigzag lattice formation, since an atomic layer of B has considerably more surface energy than the one comprised of N atoms [6]. In fact, in the formation process of σ bonds of BN nanotubes, considerable charge transference would take place between the B atoms and the nearest N atoms because of their different electronegativities (2.04 eV and 3.04 eV, respectively). This makes the distribution of charge density along the BN nanotube more nonuniform. In addition, the effect of isolated electron pairs localized at the N atoms or localized π electronic states in BN nanotubes quite substitute for that of the delocalized π electronic states in carbon nanotubes. These two inherent differences between BN and carbon nanotubes can give rise to their different physical, chemical, and mechanical properties [7]. Another effect of ionic bonds may be destabilizing single-wall nanotube formation and strengthening so-called "lip–lip" interactions between adjacent layers in multiwalled (MW) BN nanotubes [8]. So the mechanical properties of BN nanotubes can be predicted as well as those of carbon nanotubes.

Several experimental and computational methods have been used to explain the mechanical properties of BN nanotubes, yet the results have not been systematically compared. To the authors' knowledge, this is the first review of the mechanical properties of BN nanotubes. Our goal is to provide a better understanding on the relationships between the mechanical properties and structural characteristics of BN nanotubes. A more thorough review on the electrical, optical, and thermal properties of BN nanotubes was discussed in a recent article [9]; hence, they are not reviewed here.

2 Thermal Vibrations of BN Nanotube

Chopra and Zettl [10] were the first to measure the elastic modulus of individual BN nanotubes grown by the arc discharge method. The tests were performed inside a high-resolution transmission electron microscope (HRTEM) equipped with a thermal excitation apparatus. With the thermal vibration method, increasing the temperature of the specimen results in vibration. Figure 2 shows TEM images of two BN nanotubes during thermal vibration experiments. As shown, the tip of the longer one is not in focus, which is due to higher amplitude of the thermal vibration. This was verified by performing a focusing plane and rotation study. Figure 3 shows the root mean square (rms) transverse nanotube vibration amplitude as a function of distance from the nanotube base, determined from a deconvolution of the intensity line scans from the base line scan. As expected, the vibration amplitude increases with increasing distance from the clamped base of the nanotube.

The magnitude and functional form of the vibration amplitude data in Fig. 3 allowed an explicit determination of the elastic properties of BN nanotubes. The authors approximated the nanotube as a cantilever beam with a uniform circular cross section of outer diameter

$$\omega_n = (\beta_n L)^2 \sqrt{\frac{YI}{\mu L^4}} \tag{1}$$

where ω_n is the frequency, Y is the Young's modulus, and $\beta_n = 1.8751$, 4.6941, 7.8548, and 10.996 for $n=1$, 2, 3, and 4 respectively. Furthermore, μ is the mass per unit length, I is the moment of inertia of the tube, and L is the beam length. From the fit in Fig. 3 (solid line), the maximum RMS amplitude of oscillation was reported to be 0.8 nm. This fit, together with the measured dimensions of the nanotube ($a=3.5$ nm, $b=2.2$ nm, and $L=153.8$ nm)

Published online February 24, 2010. Transmitted by Assoc. Editor: Sarp Adali.