Eur. Phys. J. B **54**, 109–112 (2006)
DOI: 10.1140/epjb/e2006-00428-x

THE EUROPEAN PHYSICAL JOURNAL B

Transverse elasticity of multi-walled carbon nanotubes

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Received 17 January 2006 / Received in final form 23 October 2006
Published online 8 December 2006 –

Abstract. A discrete shell model is proposed to describe the radial deformation of carbon nanotubes under a hydrostatic pressure and the radial Young's modulus of (single- or multi-walled) nanotubes is obtained. It is found that the radial modulus decreases with increasing tube diameter while increases with increasing number of layers. The computational results agree well with the previous results of SWNTs and indicate that the radial modulus of carbon nanotubes is independent of the Poisson's ratio.

PACS. 61.46.Fg Nanotubes – 62.25.+g Mechanical properties of nanoscale materials

1 Introduction

Since the discovery of carbon nanotubes (CNTs) in 1991, their exceptional mechanical, electrical, and thermal properties have attracted great scientific and technological interest [1–6]. In the past several years, much effort has been made to theoretically characterize their mechanical properties that CNTs were found to be significantly stiffer than most materials ever known. As pointed out by previous experimental and theoretical studies, the Young's modulus for single-walled nanotubes (SWNTs) was found to be distributed over a wide range, from 0.5 TPa to 5.5 TPa [7–12] and for multi-walled carbon nanotubes (MWNTs) it was reported to be 1.8 ± 0.9 TPa [13]. It has also been reported that in graphite the elastic constant C_{11} in plane was 1.06 TPa, while the perpendicular elastic constant C_{33} yielded only 36 GPa [12]. Similarly, the radial Young modulus of CNTs is expected to be much smaller than the axial one. However, it has been noticed that previous studies of CNTs mainly focused on the longitudinal, or axial properties, but their radial behaviors were not very well understood. For applications in nanoelectromechanical and nanoelectronic systems, obtaining a fundamental understanding of the radial deformability of CNTs is as important as knowing the longitudinal properties. One example is that the radial deformation of CNTs may strongly affect their electrical properties [4–6].

Up to now, the experimental understanding of radial stiffness of CNTs was based on studies performed on single tube, with an unknown number of layers, and using deformations up to the nonlinear regime [14–17]. Theoretically, Reich et al. [18] used an ab initio simulation to calculate a nanotube of diameter 0.8 nm and obtained a radial modulus of about 650 GPa. To investigate the dependence of the radial modulus of SWNTs on tube diameter, Li and Chou [19] modeled the elastic deformation of SWNTs under hydrostatic pressure using a molecular structural mechanics method. SWNTs were reported to be more deformable in the radial direction than MWNTs, and their elasticity depends on tube diameter and the number of layers under compression. Therefore, further theoretical investigations of the radial modulus of MWNTs are desirable in order to gain a more quantitative understanding of their properties.

2 Model and formulation

This paper analyzes the elastic deformation of SWNTs and MWNTs under a hydrostatic pressure using a discrete shell model, and examines the variation of the radial Young's modulus with nanotube diameter.

It is widely accepted that SWNTs or MWNTs can be treated as single or concentric multiple layers of cylinder rolled up from graphite sheets. In order to investigate the elastic properties of an individual nanotube (single- or multi-walled), for simplicity we consider a MWNT, of which the outermost layer is exposed to a hydrostatic pressure. Each single nanotube is modeled as a hollow cylinder with free ends and thickness $h = 0.066$ nm, as shown in Figure 1. The stress components of a cylindrical shell under an external radial pressure can be expressed as [20–22]

$$\sigma_{rr} = -A\left(1 - \frac{B}{r^2}\right), \sigma_{\theta\theta} = -A\left(1 + \frac{B}{r^2}\right) \quad and \quad \sigma_{zz} = 0, \tag{1}$$

where r, θ and z are the three cylindrical coordinate, and A and B are two constants varying with layer in the MWNT and determined by boundary conditions. Given

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these, we obtain the deformation in the radial direction [20]

$$u_{n(r)} = -A\left(\frac{1-\nu}{Y} + \frac{1+\nu}{Y}\frac{B}{r^2}\right)r, \tag{2}$$

where $n(r)$ refers to the nth layer of the MWNT and ν is the Poisson's ratio for CNTs. Y is the longitudinal Young's modulus of SWNTs, which has two different kinds of definitions. One is to take interlayer spacing $t = 0.34$ nm [23] between graphite sheets instead of the thickness of SWNTs, and obtain the corresponding Youngs modulus $Y = 1.0$ TPa [12,24]. According to this definition, researchers treated MWNTs as assemblies of concentric shells, each representing a constituent SWNT, just like ours. But they neglected the thickness of SWNT and took the average interwall spacing to be the representative thickness for each of the concentric shells. This approximation leads to a theoretical prediction that Youngs moduli of SWNTs and MWNTs are approximately the same, and close to 1 TPa. However, the energy of such a shell is found to be about 26 times larger than that of SWNTs calculated through atomic models [25]. The other one is to use the classic formula: the bending rigidity $D_b = Yh^3/12(1-\nu^2)$ and the tensile rigidity $D_a = Yh$, and get the thickness and the longitudinal Young's modulus of SWNTs, around 0.066 nm and 5 TPa respectively, which was done by Yakobson et al. [26]. The latter treatment demonstrated remarkable success in interpreting many behaviors of SWNTs, in particular, through their MD simulations using the Tersoff-Brenner potential [26]. In the present paper, MWNTs are also teated as assemblies of concentric SWNT shells. However, instead of obtaining the Youngs moduli of MWNTs through a first principle calculation, we adopt a classical method using van de Waals force and elastic energy function to bind SWNTs together, and the behavior of the outmost SWNT is what we want to know. Thus, the definition given by Yakobson, Brabec, and Bernhole will be followed, that is, the thickness of SWNTs $t = 0.066$ nm and the corresponding longitudinal Youngs modulus $Y = 5$ TPa are used.

Now we consider a SWNT of external radius $R_{1(ex)}$ and internal radius $R_{1(in)} = R_{1(ex)} - h$. Suppose an external pressure $P_{1(ex)}$ is imposed on the external wall, setting $\sigma_{rr} = -P_{1(ex)}$ for $r = R_{1(ex)}$, and $\sigma_{rr} = 0$ for $r = R_{1(in)}$ yields A and B, which, according to equation (2), leads to a radial displacement of the external wall

$$u_{1(ex)} = -\frac{P_{1(ex)}R_{1(ex)}}{Y}\left[\frac{R_{1(ex)}^2 + R_{1(in)}^2}{R_{1(ex)}^2 - R_{1(in)}^2} - \nu\right].$$

Given this, the radial Young's modulus is

$$E_r^1 = \frac{P_{1(ex)}}{\frac{|u_{1(ex)}|}{R_{1(ex)}}} = \frac{Y}{\frac{R_{1(ex)}^2+R_{1(in)}^2}{R_{1(ex)}^2-R_{1(in)}^2} - \nu}.$$

A MWNT can be thought of as a number of abovementioned concentric SWNTs of different radii grouped around the central axis. $h = 0.066$ nm, as mentioned above, is the effective wall thickness of each SWNT and $d = 0.34$ nm [23] is the distance between adjacent layers of the MWNT. Suppose $R_{i(in)}$ and $R_{i(ex)}$ are the internal and the external radius of the ith layer of the MWNT respectively, as shown in Figure 1, we have

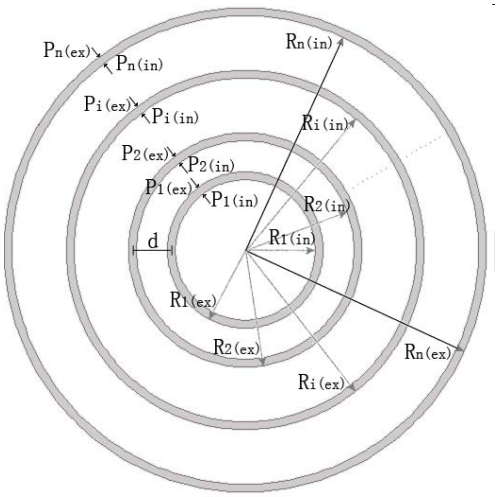

Fig. 1. Cross section of a MWNT. The adjacent layer is a distance d apart.

$$R_{i(in)} = R_{i(ex)} - h, \tag{3}$$

$$R_{i(in)} = R_{i-1(in)} + d. \tag{4}$$

The van der Waals force between adjacent carbon layers requires [27]

$$P_{i(in)}R_{i(in)} = P_{i-1(ex)}R_{i-1(ex)}. \tag{5}$$

On the other hand, once an external hydrostatic pressure is applied to an n-layer MWNT, the deformation of the MWNT leads to an elastic energy F_n defined as

$$F_n = 2\pi\sum_{i=1}^{n}\left(\int_{R_{n(in)}}^{R_{n(ex)}} f r dr\right), \tag{6}$$

where f is the strain energy density given by

$$f = \frac{1}{2Y}[(\sigma_{rr}^2 + \sigma_{\theta\theta}^2 + \sigma_{zz}^2) - 2\nu(\sigma_{rr}\sigma_{\theta\theta} + \sigma_{rr}\sigma_{zz} + \sigma_{zz}\sigma_{\theta\theta})]. \tag{7}$$

A minimization of the strain energy F_n

$$\frac{\partial F_n}{\partial P_{i(in)}} = 0, \quad i = 2, 3, 4\cdots n, \tag{8}$$

delivers the relationship between $P_{i(ex)}$ and $P_{i(in)}$:

$$P_{2(in)} = \frac{2\frac{R_{2(ex)}^2}{R_{2(ex)}^2-R_{2(in)}^2}}{\frac{R_{2(ex)}^2+R_{2(in)}^2}{R_{2(ex)}^2-R_{2(in)}^2} + \frac{R_{1(ex)}^2+R_{1(in)}^2}{R_{1(ex)}^2-R_{1(in)}^2}}P_{2(ex)},$$

$$P_{i(in)} = \frac{2\frac{R^2_{i(ex)}}{R^2_{i(ex)}-R^2_{i(in)}}}{\frac{R^2_{i(ex)}+R^2_{i(in)}}{R^2_{i(ex)}-R^2_{i(in)}} + \frac{R^2_{i-1(ex)}+R^2_{i-1(in)}-2R^2_{i-1(in)}(\frac{P_{i-1(in)}}{P_{i-1(ex)}})}{R^2_{i-1(ex)}-R^2_{i-1(in)}}} P_{i(ex)} \quad (3 \le i \le n), \quad (9)$$

with $P_{n(ex)} = P_0$. Combining equation (9) with equations (5) yields $P_{i(ex)}$ and $P_{i(in)}$ for all layers.

It is interesting to note that although strain energy is related to the Poisson's ratio ν, the relation between $P_{n(ex)}$ and $P_{n(in)}$ in equations (9) is independent of it. In most cases $R_{1(ex)} \gg h$ (=0.066 nm), equations (9) can be simplified as

$$P_{2(in)} = \frac{R_{2(ex)}}{R_{1(ex)} + R_{2(ex)}} P_{2(ex)}, \quad (10)$$

$$P_{i(in)} = \frac{R_{i(ex)}}{(1 - \frac{P_{i-1(in)}}{P_{i-1(ex)}})R_{i-1(ex)} + R_{i(ex)}} P_{i(ex)} \ (3 \le i \le n). \quad (11)$$

Once the connection between $P_{n(ex)}$ and $P_{n(in)}$ is built, the constants A_n and B_n of the outermost layer can also be obtained,

$$A_n = \frac{R^2_{n(ex)}P_{n(ex)} - R^2_{n(in)}P_{n(in)}}{R^2_{n(ex)} - R^2_{n(in)}},$$
$$B_n = \frac{R^2_{n(ex)}R^2_{n(in)}(P_{n(ex)} - P_{n(in)})}{R^2_{n(ex)}P_{n(ex)} - R^2_{n(in)}P_{n(in)}}. \quad (12)$$

Given the constants A_n and B_n, the radial Young's modulus is thus

$$E^n_r = \frac{P_{n(ex)}}{\mid u_{n(ex)} \mid / R_{n(ex)}}, \quad (13)$$

where $u_{n(ex)}$ is the radial displacement of the external tube given by equation (2). When $R_{1(ex)} \gg h$ (=0.066 nm), the radial Young's modulus can be reduced to

$$E^n_r = \frac{Yh}{(1 - \frac{P_{n(in)}}{P_{n(ex)}})R_{n(ex)}}, \quad (14)$$

which is also independent of the Poisson's ratio ν.

3 Results and discussion

Figure 2 shows the radial Young's modulus of a SWNT as a function of external diameter of the tube with different values of ν, used by different researchers [12,24,26]. It is found that the radial Young's modulus decreases with increasing external diameter, but responds little to the values of ν. More precisely, the radial modulus increases dramatically for tubes with external diameter smaller than 2 nm, and levels off to 36 GPa in the larger diameter, as can be seen in Figure 3 (lower most curve). The theoretical evaluation using the present model agrees quantitatively well with the previous experimental [15] or theoretical [18,19] results, which are also shown in Figure 2

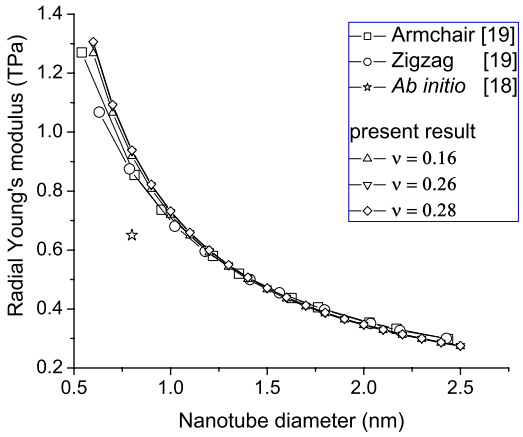

Fig. 2. Radial Young's modulus of SWNTs in transverse directions.

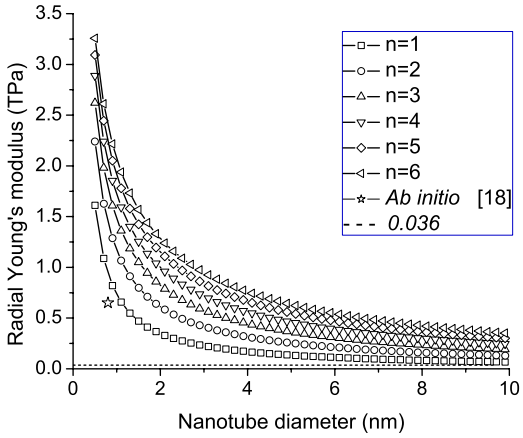

Fig. 3. Radial Young's modulus of MWNTs in transverse directions.

as data-points. The variations of the radial Young's modulus for MWNTs with number of layers are plotted in Figure 3. As can be seen, the larger the number of layers of the tubes, the stiffer they are. And the radial Young's modulus sharply decreases with the increase in diameter for MWNTs at constant number of layers, which is consistent with the previous result obtained for SWNT. This is reasonable if we consider the elastic energy necessary to roll up from a graphite sheet and the van der Waals forces between adjacent layers, which has been confirmed by experiments [28].

Here it is necessary to point out that our results in Figure 3 are a bit larger than those obtained by experiment [28]. This is understandable because our simulation is based on the model under a homogeneous hydrostatic pressure in the transverse plane, which is different from the setup in the experiment, using a scanning probe microscope or tapping-mode atomic force microscope. The MWNTs in the experiments as carried out by Palaci et al. were exposed to a uni-directional force using a cantilever of the atomic force microscope (AFM), which is actually not a pressure strictly in radial direction. The transverse

modulus obtained by this means is thus smaller than our results as it is always easier to deform a tube using a unidirectional force than a transversely homogeneous one.

4 Summary

In summary, this paper predicts the radial Young's modulus of SWNTs and MWNTs under a hydrostatic pressure using a discrete shell model to describe the radial deformation of CNTs. The computational results indicate that the radial modulus decreases with increasing tube diameter while increases with increasing the layers' number, but is independent of Poisson's ratio.

This work is supported by the National Science Foundation of China under Grant Nos. 10225420, 90206039 and 20021002.

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