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International Journal of Solids and Structures 43 (2006) 254–265
INTERNATIONAL JOURNAL OF SOLIDS and STRUCTURES
www.elsevier.com/locate/ijsolstr

Wave characteristics of carbon nanotubes

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Received 23 August 2004; received in revised form 24 February 2005
Available online 9 April 2005

Abstract

The research in the manuscript studies the wave characteristics in carbon nanotubes (CNTs) via beam theories. First, the material properties used in the beam models for the analysis of CNTs are proposed from the discrete atomic nature of CNTs. Secondly, the comparison of wave solution in a single walled carbon nanotube (SWNT) by Euler–Bernoulli beam model and Timoshenko beam model is conducted. The applicability of the two beam models is discussed from the numerical simulations. In addition, the difference of the two beam models on the terahertz frequency range is presented to show the significance of applying an appropriate continuum model in studying the wave propagation in CNTs. Thirdly, Timoshenko beam model is employed to study the wave propagation in a double walled carbon nanotube (DWNT) via a simple single beam theory by assuming co-axial motion of the two tubes, and a double beam theory accounting for van der Waals. The size effect of the DWNT on the wave solution by different beam theories is discussed as well. The feasibility of applying the simple single beam theory and the double beam theory is discussed through numerical simulations. It is hoped that the research in the manuscript may present a benchmark in the study of wave propagations in carbon nanotubes.

Keywords: Carbon nanotubes; Bending rigidity; Wave propagation; Continuum models; Phase velocity; Cut-off frequency; Timoshenko beam model

1. Introduction

Extensive researches on carbon nanotubes (CNTs) have been conducted (Ball, 2001; Baughman et al., 2002) since CNTs were discovered by Iijima (1991). Many applications of CNTs have been reported, such

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0020-7683/$ - see front matter
doi:10.1016/j.ijsolstr.2005.02.047

as atomic-force microscope (AFM), field emitters, nano-fillers for composite materials, nanoscale electronic devices. Multi-walled nanotubes (MWNTs) have the potential for the development of frictionless nano-actuators, nano-motors, nano-bearings, and nano-springs (Lau, 2003). Therefore, the researches on CNTs may lead to new applications of MEMS and other smart materials and structures. Since molecular simulations (Li and Chou, 2003; Iijima et al., 1996; Yakobson et al., 1997) are very expensive especially for large-scale problems, continuum models for CNTs have become an important tool in studying CNTs. Most of the work in this category is focused on the application of elastic shell and beam models. Yakobson et al. (1996) noticed the unique features of fullerenes and developed a continuum shell model in studying different instability patterns of a carbon nanotube under different compressive load. Ru (2000a,b) further carried on the buckling analysis of carbon nanotubes with shell models. Parnes and Chiskis (2002) investigated elastic buckling of layered/fiber-reinforced composite with elastic beam model. Krishnan et al. (1998) estimated the Young's modulus of singled-walled carbon nanotubes by observing their freestanding room-temperature vibrations in a transmission electron microscope. The nanotube dimensions and vibration amplitude are measured from electron micrographs, and it is assumed that the vibration modes are driven stochastically and are chosen of a clamped cantilever. Wang (2004) proposed the effective in-plane stiffness and bending rigidity of armchair and zigzag carbon nanotubes through the analysis of a representative volume element of the graphene layer via continuous elastic models. Yoon et al. (2003a) studied resonant frequencies and the associated vibration modes of an individual multi-walled carbon nanotube embedded in an elastic medium.

Recently, growing interest in terahertz physics of nanoscale materials and devices (Sirtori, 2002; Jeon and Kim, 2002; Antonelli and Maris, 2002; Knap et al., 2002; Brauns et al., 2002) opens a new topic on wave characteristics of CNTs, especially on the terahertz frequency range. Some researches have been reported for this topic, but mainly for SWNTs (Yu et al., 1995; Popov and Doren, 2000; Reulet et al., 2000). Yoon et al. (2003b) studied the wave propagation of DWNT and multiple walled carbon nanotubes. In their studies, van der Waals force is modeled via their multiple-beam theory. Nevertheless, Euler–Bernoulli beam model was used in almost all of the existed references in the analysis of CNTs. The applicability of this simple beam model has not been investigated so far. During the revision of the current manuscript, the authors found a recent work by Yoon et al. (2004) to study the rotary inertia and shear deformation on transverse wave propagation in CNTs. Some fundamental characteristic wave results for MWNTs were listed in their work.

In structural analysis of one-dimensional beam-like structures, two models are usually employed, namely Euler–Bernoulli and Timoshenko beam models. Both models assume that plane sections remain plane. But in Euler beam model, the sections remain perpendicular to the neutral axis whereas this assumption is removed in Timoshenko beam model (1921) to account for the effect of shear and rotary effect. Euler–Bernoulli beam model normally provides over-estimated wave phase velocity at higher wavenumber. Timoshenko model, on the other hand, is proved to be able to provide more accurate wave solution even at higher frequency range, although it is more complicated than Euler–Bernoulli model. To investigate the feasibility of the two beam models in analysis of wave propagation of CNTs on terahertz frequency range is crucial to study the wave characteristics of CNTs for their physical applications.

The research in the manuscript first proposes the derivation of material properties of CNTs used in beam models. Secondly, the research aims to study wave characteristics in a single walled carbon nanotube (SWNT) by Euler–Bernoulli beam model and Timoshenko beam model. The applicability of the two beam models is discussed from the numerical simulations. The feasibility of Euler–Bernoulli beam model is to be specially discussed on the terahertz frequency range. Thirdly, Timoshenko beam model is applied to study the wave propagation in a double walled carbon nanotube (DWNT) via a simple single beam theory by assuming co-axial motion of the two tubes, and a double beam theory accounting for van der Waals force in the model. The size effect of the DWNT is discussed from numerical simulations for the applicability of the simple single beam theory.

2. The material properties of carbon nanotubes in beam models

A key issue of applying continuum beam models in static and dynamic analyses of CNTs is the determination of materials properties of CNTs, such as the bending rigidity and mass expression of unit length in beams. As atomic structure of CNTs is of discrete nature not as what we proposed in beam structures, the derivation of all the material properties in beam models from continuous structural mechanics cannot be directly applied to the study of CNTs. The materials properties for CNTs obtained hereinafter will be used in deriving the wave characteristics of CNTs via both Euler–Bernoulli beam model and Timoshenko beam model in next sections.

The proposition for the material properties used in continuum beam models for wave propagation in CNTs will be studied through an analysis of a single walled nanotube shown in Fig. 1. The length of the SWNT is L, and the diameter of the mid-surface is d. The classical expression for the stiffness of the beam structure is given below:

$$EI = \frac{E\pi}{64}\left(d_o^4 - d_i^4\right), \tag{1}$$

where d_o and d_i are the diameters of outer and inner surfaces of the beam; $h = (d_o - d_i)/2$ is the thickness of the nanotube layer ($h = t = 0.34$ nm for a SWNT; $h = Nt$ for a N-layered MWNT); t (0.34 nm) is the equilibrium interlayer spacing of adjacent nanotubes; E is the Young's modulus of nanotube; $v = 0.145$ is the Poisson ratio.

Ru (2000a) proposed that the effective bending rigidity of a SWNT should be regarded as an independent material parameter not related to the equilibrium thickness by the elastic bending stiffness formula. Actually in all the lower-order models for beams, plates and shells, the common assumption used is the "straight normal postulate" which states that the longitudinal deformation at any point in the flexural direction is proportional to the distance between this point to the mid-plane of mid-surface of the structure. However, the atomic layer in a SWNT cannot be divided into different layers and the flexural strain or deformation are actually concentrated on a narrow region around the center-line of the atom layer, rather than distributed linearly over the thickness direction (Ru, 2000a).

The derivation of flexural stiffness is the key to the study of CNTs via beam models. Previous studies (Krishnan et al., 1998; Wong et al., 1997) used the straight normal postulate to calculate the bending stiffness of nanotubes. Based on the above discussion, it is inappropriate to assume this straight normal

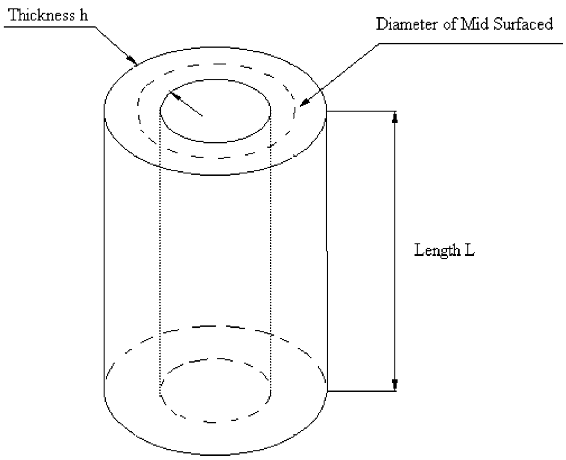

Fig. 1. Layout of a single-walled carbon nanotube.

postulate directly in the analysis since the hypothesis that the flexural stresses and deformation in a nanotube mainly concentrate on a narrow region around the central surface is also valid for the cylinder-like beam structure. Inspired by the above statement, we propose the flexural stiffness of the cylinder-like nanotube beam hereinafter.

From the results by Yakobson et al. (1996), the representative thickness of the nanotube layer is 0.066 nm which is much smaller than the diameter of most of CNTs. Substituting the equality $d_o - d_i = 2h$ and $d_o \approx d_i \approx d$ if the representative thickness of nanotube layer is very small, the stiffness of the nanotube beam structure can be expressed as follows:

$$EI = \frac{E\pi}{64}\left(d_o^4 - d_i^4\right) = \frac{\pi Eh}{8}d^3 = \frac{\pi C}{8}d^3, \tag{2}$$

where the in-plane stiffness is $Et = C = 360\ \text{J/m}^2$ (Yakobson et al., 1996) which is a virtually constant parameter. It has to be noted that although the above expression is proposed under the assumption of $d \gg h$, the error in the derivation will still be less than 4.5% if a SWNT with diameter $d = 1$ nm is investigated as the representative thickness is set 0.066 nm.

In this equation, the hypothesis of stress distribution in a small domain around the center-line is imposed and the result shows that the bending stiffness of a nanotube is proportional to the cube of the diameter of the mid-surface of the cylinder and related to the in-plane stiffness of the CNT.

The validation of this proposed stiffness has been conducted by comparing the frequencies of a cantilever SWNT results from the flexural stiffness in Eq. (2) and the experimental results by Krishnan et al. (1998) and by Wang and Varadan (2005).

The mass density of per unit length of a SWNT, ρA, has also to be proposed in the analysis of wave propagation in CNTs. $\rho = 2.3\ \text{g/cm}^3$ (Yoon et al., 2004) was proposed as the mass density of nanotube; $A = \pi dt$ is the cross area of the nanotube. Since a SWNT is rolled up from a sheet of graphite, the value of thickness in calculating the cross area of the CNT should be used from the equilibrium interlayer spacing of adjacent nanotubes, i.e. $t = 0.34$ nm.

Another two parameters used in Timoshenko beam model are GI and GA, where $G = \frac{E}{2(1+v)}$ is the shear modulus of CNTs. From previous analysis on the bending rigidity and the proposed in-plane stiffness of CNTs, the above two parameters can be proposed as follows:

$$GI = \frac{EI}{2(1+v)} = \frac{\pi C}{16(1+v)}d^3, \tag{3}$$

$$GA = \frac{Et\pi d}{2(1+v)} = \frac{C\pi d}{2(1+v)}. \tag{4}$$

Since two tubes share one center for cross area and the area moment of inertia of the cross section, the above parameters used in a doubled walled nanotube will thus be easily derived as follows:

$$EI = \frac{\pi C}{8}\left(d_1^3 + d_2^3\right), \tag{5}$$

$$\rho A = \pi\rho t(d_1 + d_2), \tag{6}$$

$$GI = \frac{\pi C}{16(1+v)}\left(d_1^3 + d_2^3\right), \tag{7}$$

$$GA = \frac{Et\pi d}{2(1+v)} = \frac{C\pi(d_1 + d_2)}{2(1+v)}, \tag{8}$$

where d_1 is the mid-surface diameter of the inner tube, and $d_2 = d_1 + 2 \times 0.34$ nm is the mid-surface diameter of the outer tube.

In the next session, Euler–Bernoulli beam model and Timoshenko beam model will be applied to study the wave propagation in a SWNT.

3. Wave characteristics of SWNTs by two beam models

Two beam models are usually used in flexural motion analysis of one-dimensional structures in structural mechanics, namely Euler–Bernoulli and Timoshenko beam models. Both models assume that plane sections remain plane but in Euler beam model, the sections remain perpendicular to the neutral axis whereas this assumption is removed in Timoshenko beam model (1921) to account for the effect of shear and rotary inertia. In the Euler beam model, the effects of rotary inertia and shear deformation are neglected. Timoshenko (1921) included both effects of shear and rotary inertia and obtained results of wave propagation in better agreement with those using exact theory. The investigation of the feasibility of the two beam models in the analysis of wave propagation of CNTs will be conducted next.

The governing equation for the SWNT from Euler–Bernoulli beam model is given as

$$EI\frac{\partial^4 u}{\partial x^4} + \rho A\frac{\partial^2 u}{\partial t^2} = 0, \tag{9}$$

where $u(x,t)$ is the flexural deflection of the beam structure. The wave propagation solution of Eq. (9) can be expressed as follows:

$$u(x,t) = U\,\mathrm{e}^{\mathrm{i}(kx-\omega t)}, \tag{10}$$

where U is the amplitude of the wave motion, k is the wavenumber, and ω is the frequency of the wave motion.

Substitution of Eq. (10) into Eq. (9) yields,

$$\left(EIk^4 - \rho A\omega^2\right)U = 0, \tag{11}$$

from which the wave characteristic phase velocity, $v = \omega/k$, is derived as,

$$v = k\sqrt{\frac{EI}{\rho A}}. \tag{12}$$

The phase velocity of the SWNT by Euler–Bernoulli beam theory can be derived as follows by substituting the expressions of bending rigidity and mass per unit length of the SWNT,

$$v = k\sqrt{\frac{Cd^2}{8\rho t}}. \tag{13}$$

The governing equation for the SWNT from Timoshenko beam model is given as

$$GA\kappa\left(\frac{\partial\varphi}{\partial x} - \frac{\partial^2 u}{\partial x^2}\right) + \rho A\frac{\partial^2 u}{\partial t^2} = 0, \tag{14}$$

$$GA\kappa\left(\frac{\partial u}{\partial x} - \varphi\right) + EI\frac{\partial^2\varphi}{\partial x^2} - \rho I\frac{\partial^2\varphi}{\partial t^2} = 0, \tag{15}$$

where φ is introduced to measure the slope of the cross-section due to bending, κ is the adjustment coefficient which is suggested to take as 10/9 for a circular shape of the cross area (Graff, 1975). Since in nanotube model, the equivalent thickness of the tube is very small as discussed before, the term for rotary inertia, $\rho I\frac{\partial^2\varphi}{\partial t^2}$, can be neglected in the calculation.

A single equation can be reduced by a simple calculation to eliminate the term φ in the above two equations shown below,

$$\frac{Cd^2}{8\rho t}\frac{\partial^4 u}{\partial x^4} - d^2\left(\frac{1+v}{4\kappa}+\frac{1}{8}\right)\frac{\partial^4 u}{\partial x^2\,\partial t^2} + \frac{\partial^2 u}{\partial t^2} = 0. \tag{16}$$

Substitution of the harmonic wave solution in Eq. (10) in Eq. (16) leads to the expression of phase wave velocity via Timoshenko beam model for the SWNT as follows:

$$v = \sqrt{\frac{Cd^2k^2}{8\rho t + 8\rho t d^2\left(\frac{1+v}{4\kappa}+\frac{1}{8}\right)k^2}}. \tag{17}$$

In Fig. 2(a), the natural logarithmic calculation of wave phase velocity versus the wavenumber from the two models is platted. It is clearly seen that at lower wavenumber ($k < e^{20} \approx 4\times10^8$), the two beam models provide almost the same solution for the wave phase velocity. On the other hand, Euler–Bernoulli model shows the linear relation of the two variables, also seen in Eq. (13), whereas, Timoshenko model displays non-dispersive wave characteristic, i.e. constant phase wave velocity, at higher frequency range, i.e. $k > 4\times10^8$. In Fig. 2(b), the natural logarithmic calculation of the frequency of the wave motion versus the wavenumber is provided. It is seen that the Euler–Bernoulli model provides higher estimate of the

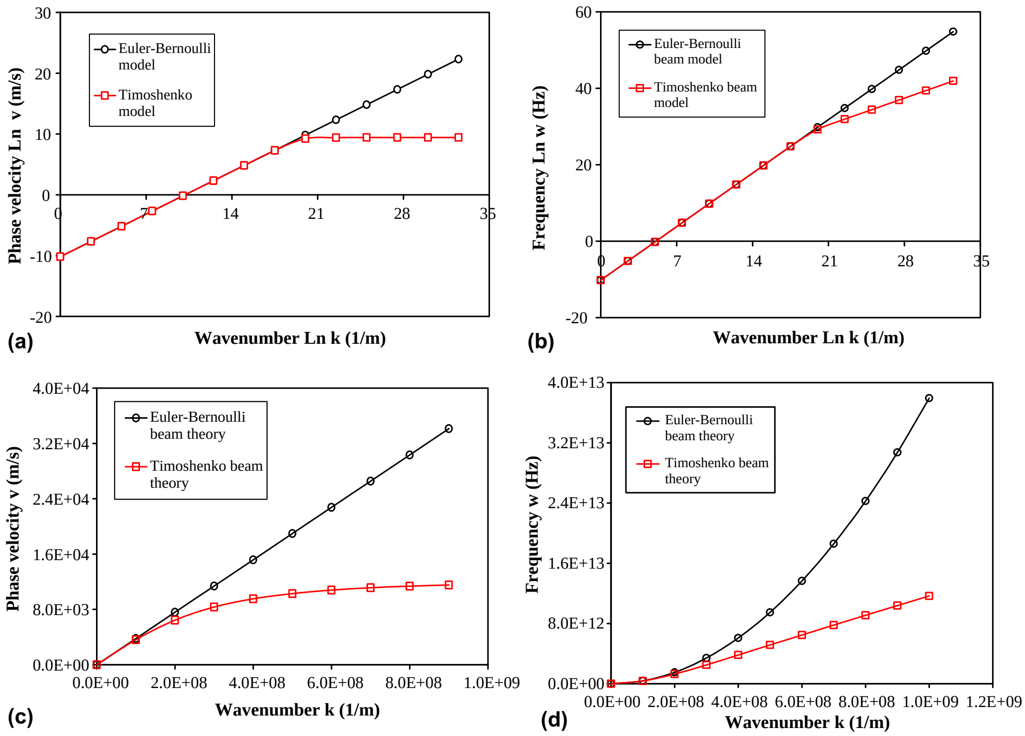

Fig. 2. (a) Comparison of phase velocity from two beam models. (b) Comparison of dependent frequency by two beam models. (c) Wave phase velocity in the THz range. (d) Wave characteristic in the range of THz.

frequency value at wavenumber above $k > 4 \times 10^8$. The frequency range for the feasibility of Euler–Bernoulli beam model is found to be around $\omega > 1$ THz. The zoom-in layout of the wave phase velocity and frequency at the range of $k = 10^8$–10^9 is provided in Fig. 2(c) and (d), from which the difference of the two beam theories is clearly observed. As discussed in introduction, rapidly growing interest in terahertz physics of nanoscale materials and devices arises open problems in wave propagation in CNTs on terahertz frequency range. From the above numerical simulations, Euler–Bernoulli model is not an appropriate beam model in the analysis of wave propagation of CNTs as the wave solution based on this theory deviates far from that predicted by Timoshenko model on the terahertz frequency range.

In the next section, the wave propagation in a DWNT will be studied via Timoshenko beam model.

4. Wave characteristics of double walled carbon nanotubes

The single beam theory was widely used in the references (Wong et al., 1997; Falvo et al., 1997; Treacy et al., 1996; Poncharal et al., 1999). In the analysis of a DWNT, single beam model assumes the two tubes of the DWNT remain coaxial during deformation. Definitely, this is a simpler theory and the wave propagation in the DWNT can be directly derived from the above solution for SWNTs. However, this theory cannot take into account of the van der Waals interaction effect at the interface of the inner and outer tubes of the DWNT. How to evaluate the effect of van der Waals force on the wave solution in DWNTs will be studied next. The double beam theory, or multiple beam theory (Yoon et al., 2003b), will model the van der Waals effect in the modeling of the wave propagation in DWNTs. Since Timoshenko beam model is appropriate to study the wave propagation in CNTs on terahertz range, this beam model will be used to study the wave characteristics in a DWNT via single beam theory and double beam theory respectively.

In linear analysis, the van der Waals interaction pressure at any point between two adjacent tubes was modeled by a linear function of the deflection jump at that point (Yoon et al., 2003a). In terms of the above model of the van der Waals interaction, the governing equations for the inner and outer tubes can be written as follows via Timoshenko beam model:

$$(GA)_1\kappa\left(\frac{\partial\varphi_1}{\partial x} - \frac{\partial^2 u_1}{\partial x^2}\right) + \rho A\frac{\partial^2 u_1}{\partial t^2} = c(u_2 - u_1), \tag{18a}$$

$$(GA)_1\kappa\left(\frac{\partial u_1}{\partial x} - \varphi_1\right) + (EI)_1\frac{\partial^2\varphi_1}{\partial x^2} - (\rho I)_1\frac{\partial^2\varphi_1}{\partial t^2} = 0, \tag{18b}$$

$$(GA)_2\kappa\left(\frac{\partial\varphi_2}{\partial x} - \frac{\partial^2 u_2}{\partial x^2}\right) + (\rho A)_1\frac{\partial^{2_1} u_2}{\partial t^2} = -c(u_2 - u_1), \tag{19a}$$

$$(GA)_2\kappa\left(\frac{\partial u_2}{\partial x} - \varphi_2\right) + (EI)_2\frac{\partial^2\varphi_2}{\partial x^2} - (\rho I)_2\frac{\partial^2\varphi_2}{\partial t^2} = 0, \tag{19b}$$

where the subscript 1 and 2 stand for the variables in inner and outer tubes respectively.

The evaluation of the constant c was suggested by Yoon et al. (2003a) as which is $c \approx \frac{320(2\bar{r})\mathrm{erg/cm}^2}{0.16a^2}$ and $\bar{r} = \frac{1}{4}(d_1 + d_2)$, $a = 1.42 \times 10^{-8}$ cm. It has to be noted that the constant should be dependent on the curvature of CNTs (Yoon et al., 2003a; Wang et al., 2005). From viewpoint of structural mechanics, the effect of the van der Waals force is like distributed spring with stiffness c attached at the interface of the inner and outer tube of this DWNT.

Following the similar manipulations in Eqs. (14) and (15) and ignoring the rotary inertia effect, the wave motion in the DWNT via the double beam theory can be governed by,

$$\frac{(EI)_1}{(\rho A)_1}\frac{\partial^4 u_1}{\partial x^4}-\frac{(GI)_1\kappa+(EI)_1}{(GA)_1\kappa}\frac{\partial^4 u_1}{\partial x^2\,\partial t^2}+\frac{\partial^2 u_1}{\partial t^2}+\frac{c}{(GA)_1\kappa}\left(-\frac{(GA)_1\kappa}{(\rho A)_1}(u_2-u_1)+\frac{(EI)_1}{(\rho A)_1}\left(\frac{\partial^2 u_2}{\partial x^2}-\frac{\partial^2 u_1}{\partial x^2}\right)\right)=0, \tag{20}$$

$$\frac{(EI)_2}{(\rho A)_2}\frac{\partial^4 u_2}{\partial x^4}-\frac{(GI)_2\kappa+(EI)_2}{(GA)_2\kappa}\frac{\partial^4 u_2}{\partial x^2\,\partial t^2}+\frac{\partial^2 u_2}{\partial t^2}+\frac{c}{(GA)_2\kappa}\left(-\frac{(GA)_2\kappa}{(\rho A)_2}(u_1-u_2)+\frac{(EI)_2}{(\rho A)_2}\left(\frac{\partial^2 u_1}{\partial x^2}-\frac{\partial^2 u_2}{\partial x^2}\right)\right)=0. \tag{21}$$

The wave solutions for inner and outer tubes are expressed in the harmonic forms as follows:

$$u_1(x,t)=U_1\,\mathrm{e}^{\mathrm{i}(kx-\omega t)}, \tag{22a}$$

$$u_2(x,t)=U_2\,\mathrm{e}^{\mathrm{i}(kx-\omega t)}. \tag{22b}$$

Substitution of Eqs. (22a) and (22b) into Eqs. (20) and (21) leads to the following two equations:

$$\left(\frac{(EI)_1}{(\rho A)_1}k^4-\frac{(GI)_1\kappa+(EI)_1}{(GA)_1\kappa}k^2\omega^2-\omega^2+\frac{c}{(\rho A)_1}+\frac{(EI)_1}{(\rho A)_1}k^2\right)U_1+\left(-\frac{c}{(\rho A)_1}-\frac{(EI)_1}{(\rho A)_1}k^2\right)U_2=0, \tag{23}$$

$$\left(-\frac{c}{(\rho A)_2}-\frac{(EI)_2}{(\rho A)_2}k^2\right)U_1+\left(\frac{(EI)_2}{(\rho A)_2}k^4-\frac{(GI)_2\kappa+(EI)_2}{(GA)_2\kappa}k^2\omega^2-\omega^2+\frac{c}{(\rho A)_2}+\frac{(EI)_2}{(\rho A)_2}k^2\right)U_2=0. \tag{24}$$

The wave characteristics of the DWNT can be obtained from an eigenvalue problem for searching for the non-trivial solution for U_1 and U_2 shown in the following determinant expression:

$$\begin{vmatrix}\frac{(EI)_1}{(\rho A)_1}k^4-\frac{(GI)_1\kappa+(EI)_1}{(GA)_1\kappa}k^2\omega^2-\omega^2+\frac{c}{(\rho A)_1}+\frac{(EI)_1}{(\rho A)_1}k^2 & -\frac{c}{(\rho A)_1}-\frac{(EI)_1}{(\rho A)_1}k^2\\ -\frac{c}{(\rho A)_2}-\frac{(EI)_2}{(\rho A)_2}k^2 & \frac{(EI)_2}{(\rho A)_2}k^4-\frac{(GI)_2\kappa+(EI)_2}{(GA)_2\kappa}k^2\omega^2-\omega^2+\frac{c}{(\rho A)_2}+\frac{(EI)_2}{(\rho A)_2}k^2\end{vmatrix}=0. \tag{25}$$

The cut-off frequency can be obtained by substituting $k=0$ in Eq. (25) as follows:

$$\omega=\sqrt{\frac{c(A_1+A_2)}{\rho A_1A_2}}=\sqrt{\frac{c(d_1+d_2)}{\rho\pi t d_1 d_2}}. \tag{26}$$

The asymptotic solution for the wave phase velocity of the DWNT can be obtained from Eq. (25) by assuming $k\to\infty$, and is derived as,

$$\left(\frac{(EI)_1}{(\rho A)_1}-\frac{(GI)_1\kappa+(EI)_1}{(GA)_1\kappa}v^2\right)\left(\frac{(EI)_2}{(\rho A)_2}-\frac{(GI)_2\kappa+(EI)_2}{(GA)_2\kappa}v^2\right)=0, \tag{27}$$

from which the two asymptotic velocities goes to the same value,

$$v_{1s}=v_{2s}=\sqrt{\frac{\frac{(EI)_1}{(\rho A)_1}}{\frac{(GI)_1\kappa+(EI)_1}{(GA)_1\kappa}}}=\sqrt{\frac{\frac{(EI)_2}{(\rho A)_2}}{\frac{(GI)_2\kappa+(EI)_2}{(GA)_2\kappa}}}=\sqrt{\frac{C}{8\rho t\left(\frac{1+v}{4\kappa}+\frac{1}{8}\right)}}, \tag{28}$$

which is the asymptotic solution for the wave motion of SWNT shown in Eq. (17) by Timoshenko theory. The asymptotic velocity is around 12,250 m/s for a DWNT with inner radius 3.5 nm, whereas the result is 11,795 m/s predicted by Yoon et al. (2004). The difference is only 3.7%.

It is seen that there are two wave motion modes. The explicit expressions of the phase velocities of the two wave modes can be derived from Eq. (25) as follows:

$$v_1 = \frac{Q}{2P} - \frac{\sqrt{Q^2 - 4PR}}{2P}, \tag{29}$$

$$v_2 = \frac{Q}{2P} + \frac{\sqrt{Q^2 - 4PR}}{2P}, \tag{30}$$

where

$$P = \left(\frac{(GI)_1\kappa + (EI)_1}{(GA)_1\kappa}k^4 + k^2\right)\left(\frac{(GI)_2\kappa + (EI)_2}{(GA)_2\kappa}k^4 + k^2\right),$$

$$Q = \left(\frac{(GI)_1\kappa + (EI)_1}{(GA)_1\kappa}k^4 + k^2\right)\left(\frac{(EI)_2}{(\rho A)_2}k^4 + \frac{c}{(\rho A)_2} + \frac{(EI)_2}{(\rho A)_2}k^2\right) + \left(\frac{(GI)_2\kappa + (EI)_2}{(GA)_2\kappa}k^4 + k^2\right)\left(\frac{(EI)_1}{(\rho A)_1}k^4 + \frac{c}{(\rho A)_1} + \frac{(EI)_1}{(\rho A)_1}k^2\right),$$

$$R = \left(\frac{(EI)_1}{(\rho A)_1}k^4 + \frac{c}{(\rho A)_1} + \frac{(EI)_1}{(\rho A)_1}k^2\right)\left(\frac{(EI)_2}{(\rho A)_2}k^4 + \frac{c}{(\rho A)_2} + \frac{(EI)_2}{(\rho A)_2}k^2\right) - \left(\frac{c}{(\rho A)_1} + \frac{(EI)_1}{(\rho A)_1}k^2\right)\left(\frac{c}{(\rho A)_2} + \frac{(EI)_2}{(\rho A)_2}k^2\right).$$

The mode shape of the two wave modes can be evaluated from the following expression based on Eq. (24):

$$\left(\frac{U_2}{U_1}\right)_1 = \frac{\frac{(EI)_1}{(\rho A)_1}k^4 - \frac{(GI)_1\kappa + (EI)_1}{(GA)_1\kappa}k^4 v_1^2 - k^2 v_1^2 + \frac{c}{(\rho A)_1} + \frac{(EI)_1}{(\rho A)_1}k^2}{-\frac{c}{(\rho A)_1} - \frac{(EI)_1}{(\rho A)_1}k^2}, \tag{31}$$

$$\left(\frac{U_2}{U_1}\right)_2 = \frac{\frac{(EI)_1}{(\rho A)_1}k^4 - \frac{(GI)_1\kappa + (EI)_1}{(GA)_1\kappa}k^4 v_2^2 - k^2 v_2^2 + \frac{c}{(\rho A)_1} + \frac{(EI)_1}{(\rho A)_1}k^2}{-\frac{c}{(\rho A)_1} - \frac{(EI)_1}{(\rho A)_1}k^2}. \tag{32}$$

Next, the comparison of the wave phase velocities from the single beam theory and the double beam theory will be conducted.

First, the velocities of the two wave modes from the double beam theory and the wave velocity from the single beam theory are plotted in Fig. 3(a) at $d_1 = 5$ nm. It is clearly seen that the wave velocity of the first wave mode from double beam theory is almost exactly the same with the solution from the single beam theory. On the other hand, the wave velocity of the second mode from the double beam theory decreases from very high value at lower wavenumber to the asymptotic value at higher wavenumber. The three velocities share the same asymptotic value as predicted from Eq. (28). The two mode shapes of the wave motion, i.e. $(\frac{U_2}{U_1})_1$ and $(\frac{U_2}{U_1})_2$ are shown in Fig. 3(b). From the first curve $(\frac{U_2}{U_1})_1 \approx 1$, it shows the first mode is for the motion of co-axial deflection of the DWNT for all wavenumber. The second mode shape read from the second curve $(\frac{U_2}{U_1})_2 \approx -1$, on the other hand, displays a shape of negative amplitude ratio for all wavenumber, which indicates that the deflection of the two tubes is opposite to each other with same amplitude. The conclusion from these two figures is that the single beam theory can accurately predict the first mode of the wave motion of DWNTs with larger diameter, whereas, solution for second wave mode can only be obtained from double beam theory. Therefore, if the solution for the wave motion of the first mode is the only concern, the single beam theory is appropriate for the analysis of DWNTs.

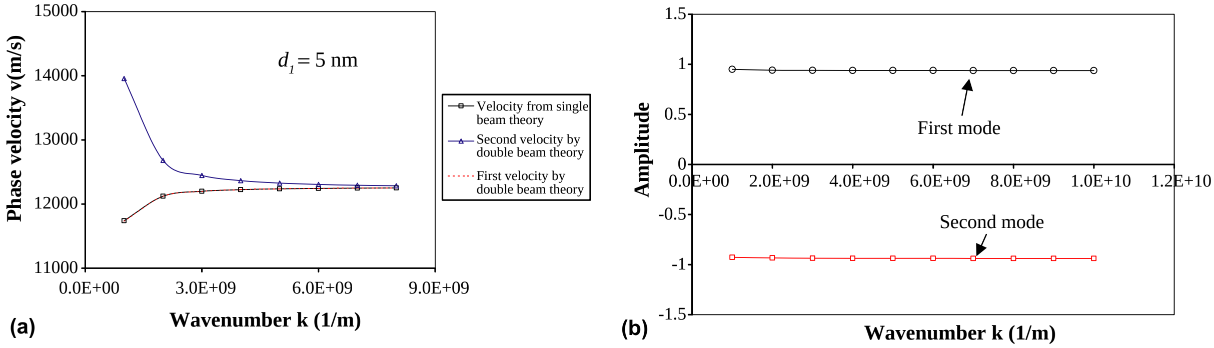

Fig. 3. (a) Comparison of the phase velocities by single beam theory and double beam theory at $d_1 = 5$ nm. (b) Mode shapes of wave propagation at $d_1 = 5$ nm.

The phase velocities from the double beam theory and the velocity from the single beam theory at $d_1 = 2$ nm are given in Fig. 4(a). The corresponding first mode shape and the second mode shape are provided in Fig. 4(b). Minor difference between the velocity for the first mode from the double beam theory and the velocity from the single beam theory is observed at lower wavenumber. At higher wavenumber, all the velocities again approach the asymptotic solution shown in Eq. (28). The conclusion can also be seen from the mode shapes in Fig. 4(a) and (b) since the ratio $\frac{U_2}{U_1}$ tends to be constant only at higher wavenumber.

Major difference between the two beam theories is clearly observed from Fig. 5(a) and (b) at smaller diameter of the DWNT $d_1 = 1$ nm. At lower wavenumber, the velocity of the first mode from the double beam theory and the velocity from the single beam theory are obviously different indicated from Fig. 5(a). The three velocities converge to the asymptotic value only at higher wavenumber. Besides, the shapes of the ratio $\frac{U_2}{U_1}$ change sharply at lower wavenumber and become stable till higher wavenumber. In addition, the asymptotic value of the two modes is not unit. The simulations in these figures show that single beam theory is inappropriate to model the wave motion of DWNTs with smaller diameter even at higher wavenumber, and the van der Waals effect must be modeled in predicting the wave characteristics of DWNTs by the double beam theory.

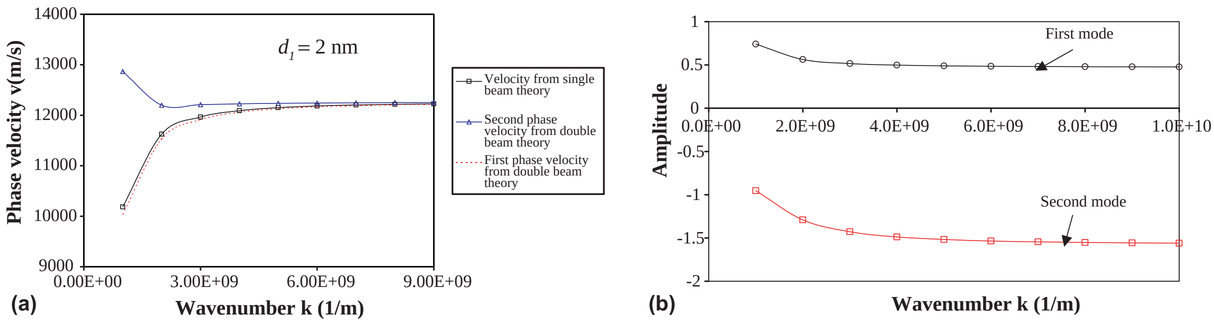

Fig. 4. (a) Comparison of phase velocities from single and double beam theories at $d_1 = 2$ nm. (b) Mode shape of wave propagation at $d_1 = 2$ nm.

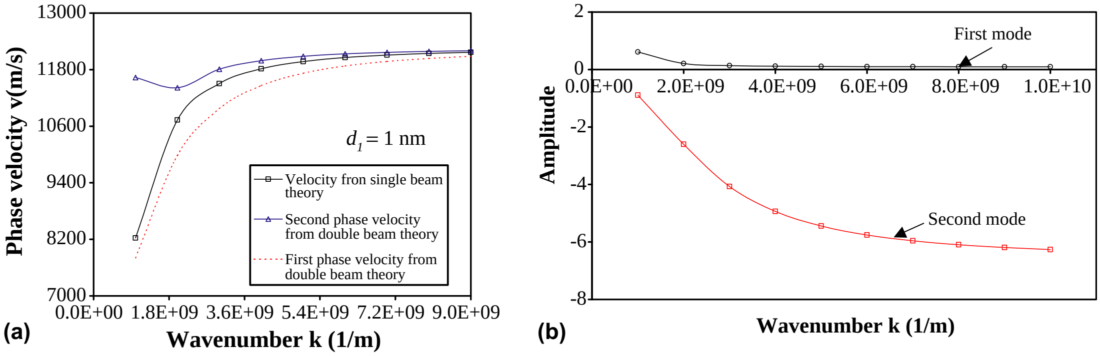

Fig. 5. (a) Comparison of phase velocities from single and double beam theories at $d_1 = 1$ nm. (b) Mode shape of wave propagation at $d_1 = 1$ nm.

5. Concluding remarks

The research in the manuscript studies the wave characteristics in carbon nanotubes via beam theories. The numerical simulations on the comparison of wave solution in a SWNT by Euler–Bernoulli beam model and Timoshenko beam model show that the Euler–Bernoulli beam model is inappropriate on the frequency range of terahertz. The Timoshenko beam model must be employed in the analysis of wave motion in CNTs, especially for the frequency range of terahertz. The research provides the modeling of wave propagation in a DWNT via a simple single beam theory by assuming co-axial motion of the two tubes, and a double beam theory accounting for van der Waals force in the model as well. The results show that the single beam theory is simple and appropriate for the analysis of DWNTs with larger diameter. For DWNTs with smaller diameter, for example, $d_1 < 2$ nm, the single beam model is not valid in predicting the wave characteristics of DWNTs, especially at lower wavenumber. On the other hand, double beam theory can provide solutions for two wave modes, whereas, single beam theory can only provide the solution for the first wave mode. At higher wavenumber, the velocities from the single beam model and double beam model approach an asymptotic value for DWNTs with higher diameter explicitly derived in the research. It is hoped that the research in the manuscript may present a benchmark in the study of wave propagations in carbon nanotubes.

Acknowledgement

Comments from one of the reviewers are highly appreciated by the authors.

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