Investigation of Wave Propagation in Multiwall Carbon Nanotubes

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Carbon nanotubes (CNTs) possess extraordinary physical properties. The fundamental understanding of nano-structure material properties and their effect on the mechanical behavior are required in order to develop reliable constitutive models for various design purposes. Since controlled experiments at nanoscales is difficult, and molecular-dynamics simulations remain formidable expense especially for large-scale systems, continuum elastic models have been widely and successfully used to study buckling、vibration and wave propagation in CNTs. MWCNTs (Multiwall Carbon Nanotubes) have been modeled as a single elastic beam which ignored non-coaxial intertube radial displacements and the related internal degrees of freedom. Ru[1] *et al* suggested a multiple-elastic-beam mode. This model is only applicable for CNTs with the certain range radius when $R_{NT}/a_{NT} \approx 1$(a_{NT} is the width of hexagonal carbon rings ,of about 0.24nm).The diameter of NTs , d_{NT} , may vary from about 0.4 to 100nm.

CNTs are novel cylindrical macromolecules composed of carbon atoms in a periodic hexagonal arrangement. The structural characteristics of CNTs make them similar to beams for CNTs with small radii, and cylindrical shells for CNTs with large radii. When L_{NT} (nanotube length)and R_{NT} (nanotube radius) are substantially larger than its maximum thickness, CNTs have some dimensional characteristics of a macroshell. The CNTs with the certain range ratio of thickness to radii (h_{NT}/R_{NT}), namely $1/1000<h_{NT}/R_{NT}<1/10$, should be considered thin shells[2].

The study of vibration and wave propagation in CNTs is one of interest of researchers. We suggest a multiple-elastic-shell model, in which each of the originally concentric nest nanotubes of MWCNTs is described using an individual elastic shell, and the deflections of all nest tubes are coupled through the van der Waals interaction between any two adjacent tubes. Transverse disturbing wave propagation in a N-wall CNT is described using the following N-couple equations.

$$
\begin{aligned}
&d_1[w_2-w_1]=2\pi R_1 D_1\frac{\partial^4 w_1}{\partial x^4}+\rho A_1\frac{\partial^2 w_1}{\partial t^2}\\
&d_2[w_3-w_2]-d_1[w_2-w_1]=2\pi R_2 D_2\frac{\partial^4 w_2}{\partial x^4}+\rho A_2\frac{\partial^2 w_1}{\partial t^2}\\
&-d_{N-1}[w_N-w_{N-1}]=2\pi R_N D_N\frac{\partial^4 w_N}{\partial x^4}+\rho A_N\frac{\partial^2 w_N}{\partial t^2},
\end{aligned}
\tag{1}
$$

where x is the axial coordinate, t is time,$w_i(x,t)(i=1,2\text{---}N)$ is the deflection of the i-th nanotube， D_i and A_i are the effective bending stiffness and the area of the cross section of the i-th tube, the subscripts1,2,.....,N are used to denote the quantities of the tube, respectively, and all tubes have the same young's modulus E=1TPa and the mass density $\rho=1.3g/cm^3$,the interaction coefficients d_i (i=1,2---N-1) can be estimated approximately

$$
d_i=\frac{200\times(2R_i)erg/cm}{0.16e^2},\qquad e=0.142nm,\quad i=1,2,\cdots,N-1
\tag{2}
$$

Consider a doublewall nanotubes (DWNT). The equation for a DWNTs is given by the two of Eq.(1) withind_2=0.Thus, for a sinusoid disturbing wave, substituting $w_1=a_1e^{i(kx-\omega t)}, w_2=a_2e^{i(kx-\omega t)}$ to Eq (1) ,the following equation can be got two wave speeds C_1 and C_2.

$$
C_1=\frac{\sqrt{2}\omega}{\sqrt{\xi+\sqrt{\xi^2-4\eta}}},\qquad C_2=\frac{\sqrt{2}\omega}{\sqrt{\xi-\sqrt{\xi^2-4\eta}}},
\tag{3}
$$

where

$$
\begin{aligned}
\xi&=\left(\frac{\rho A_1}{2\pi R_1 D_1}+\frac{\rho A_2}{2\pi R_2 D_2}\right)\omega^2-d_1\left(\frac{1}{D_1}+\frac{1}{D_2}\right),\\
\eta&=\frac{\rho^2 A_1 A_2}{(2\pi)^2 R_1 R_2 D_1 D_2}\omega^4-\frac{d_1\rho(A_1+A_2)}{(2\pi)^2 R_1 R_2 D_1 D_2}\omega^2
\end{aligned}
\tag{4}
$$

$$
\frac{a_1}{a_2}=1+\frac{2\pi R_2 D_2 k^4}{d_1}-\frac{\rho A_2\omega^2}{d_1}
\tag{5}
$$

Where a_1 and a_2 represent the amplitudes of the inner and the outer tubes, respectively. k and ω are the wave number and the circular frequency.

For the sake of comparison, the transverse wave speed of a DWNT given by the single-shell model is

$$c_o = \left(\frac{2\pi RD\omega^2}{\rho A} \right) \quad (6)$$

where D and A are the total moment of and the cross sectional area of DWNT. As $k \to 0$, the cut-off frequencies are:

$$\omega = \sqrt{\frac{(A_1 + A_2)d_1}{\rho A_1 A_2}} \quad (7)$$

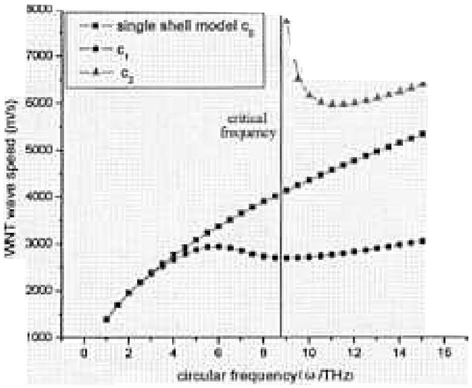

Fig.1. DWNT wave speeds vs frequency

Two wave speeds of double- wall-shell model is given in Fig.1. It is seen from Fig.1 that when the frequency is below the critical frequency , only one wave speed exists, and the associated vibration mode of the DWNT is almost coaxial. However, once the frequency exceeds the critical frequency, a non-coaxial vibration mode emerges. The two wave speeds (Eq.3) predicted by the present model are significantly different from that given by the single-shell model, and their vibration modes are substantially non-coaxial.

Further, a five-wall CNTs with the innermost diameter 3.5nm and the outermost diameter 10.0nm are discussed. In this case, Eq.(1) gives five coupled equation. There exist five critical frequencies for five-wall CNTs. They are $\omega_1 = 6.68THz$ $\omega_2 = 7.42THz$ $\omega_3 = 8.45THz$ $\omega_4 = 8.75THz$ and $\omega_5 = 5.59THz$

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respectively. Five wave speeds of five-wall CNTs are given in Fig.2, with comparison to the speed given by the single-shell model. It is seen from Fig.2 that when the frequency is below the critical frequency, only one wave

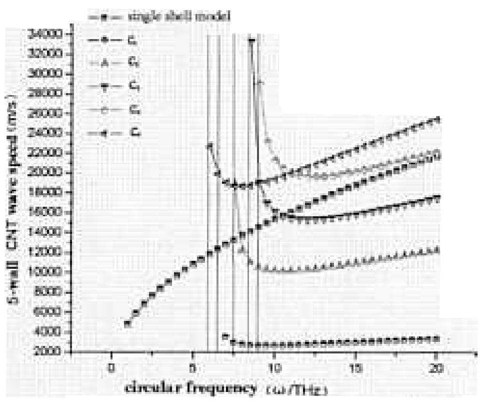

Fig.2. 5-wall CNTs wave speeds vs frequency

speed exists, and the vibration mode of the MWNT is almost coaxial. However, once the frequency exceeds one of critical frequency, a part of vibration modes is coaxial and another is non-coaxial.

These results clearly show that the single-shell model fails to predict the wave speed and vibration mode for MWNTs at ultrahigh frequencies and wave propagation in MWNTs exhibits complex phenomena and is highly non-coaxial. Therefore, wave propagation in MWNTs at ultrahigh frequencies has to be described by the present model which account for the intertube radial displacements and the related internal degrees of freedom.

Reference

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2. V. M. Harik, Mechanics of carbon nanotubes: applicability of the continuum beam models, Computational materials science, 24 (2002) 328—342.