Noncoaxial resonance of an isolated multiwall carbon nanotube

J. Yoon, C. Q. Ru,* and A. Mioduchowski
Department of Mechanical Engineering, University of Alberta, Edmonton, Canada T6G 2G8

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This brief report studies noncoaxial mechanical resonance of an isolated multiwall carbon nanotube. Noncoaxial resonant frequencies and the associated noncoaxial vibrational modes are calculated. For shorter or periodically supported multiwall carbon nanotubes, the lowest noncoaxial resonant frequencies predicted by the present model are comparable to their first few higher natural frequencies, which indicates that noncoaxial resonance will be excited at the higher natural frequencies. Since noncoaxial vibration will distort otherwise concentric geometry of multiwall carbon nanotubes, it could crucially affect their physical (such as electronic and optical) properties.

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Carbon nanotubes (CNT's) hold substantial promise as building blocks for nanoelectronics, nanodevices, and nanocomposites,[1–8] because of their electronic and mechanical properties. Mechanical behavior of CNT's has been the subject of much recent research. Since controlled experiments at the nanometer scale are difficult, and molecular-dynamics simulations remain formidable for large-scale systems, continuum elastic models have been widely and successfully used to study mechanical behavior of CNT's, such as static deflection, thermal vibration, and resonant frequencies.[9–12] In particular, the single-elastic beam model,[10–12] which ignores intertube radial displacements and the related internal degrees of freedom, has been widely used to study mechanical behavior of multiwall nanotubes (MWNT's).[3–6,13] As shown in Ref. 14 for column buckling of MWNT's, such a simplified model is adequate for free-standing MWNT's of a larger aspect ratio.

However, in many proposed designs of singlewall-nanotube- (SWNT) or MWNT-based electronics and nanodevices, see, e.g., Refs. 1–4, CNT's are often supported periodically. In some other applications, such as nanotweezers and antiferromegnetic AFM tips,[7,8] shorter CNT's are preferred to prevent undesirable kinking and buckling. Therefore, vibrational behavior of shorter or periodically supported MWNT's is of practical interest. In these cases, it is anticipated that intertube radial displacements of MWNT's would come to play a significant role and give rise to different resonant frequencies and noncoaxial vibrational modes. Although noncoaxial intertube vibration would not substantially affect the overall deflection of MWNT's, it could distort otherwise concentric geometry and thus crucially affect some of their physical (especially electronic[15–18] and optical[19,20]) properties. Hence, it is relevant to study when vibration of MWNT's becomes essentially noncoaxial.

The existing single-beam model[9–12] assumes that all nested individual tubes of a MWNT remain coaxial during vibration and thus can be described by a single deflection curve. Evidently, such a model cannot be used to study noncoaxial intertube vibrations of MWNT's. Here, a multiple-elastic beam model is suggested, in which each of the nested nanotubes is described as an individual elastic beam, and the deflections of all nested tubes are coupled through the van der Waals interaction between any two adjacent tubes. Since all nested tubes are originally concentric and the van der Waals interaction depends on the intertube spacing, the net van der Waals interaction pressure remains zero for each of all nested tubes, provided they vibrate coaxially. For noncoaxial vibration, the net interaction pressure (per unit axial length) between any two adjacent tubes depends on the jump of their deflections. Here, we only consider infinitesimal vibration, and study resonant frequencies and the associated vibrational modes. Therefore, as usual, nonlinear large-deflection effects are not taken into account. In fact, as pointed out in Ref. 1, calculations using the nonlinear large-deflection model agree well with those using the computationally less costly linear small-deflection model. Thus, the net interaction pressure at any point between any two adjacent tubes linearly depends on the jump of the deflections at that point. Therefore, flexural vibration of an N-wall CNT is described by the following N coupled equations:

$$c_1[w_2-w_1]=EI_1\frac{d^4w_1}{dx^4}+\rho A_1\frac{d^2w_1}{dt^2},$$

$$c_2[w_3-w_2]-c_1[w_2-w_1]=EI_2\frac{d^4w_2}{dx^4}+\rho A_2\frac{d^2w_2}{dt^2},$$

$$\ldots\ldots$$

$$-c_{(N-1)}[w_N-w_{N-1}]=EI_N\frac{d^4w_N}{dx^4}+\rho A_N\frac{d^2w_N}{dt^2}, \qquad (1)$$

where x is the axial coordinate, t is time, $w_k(x,t)$ ($k=1,2...N$) is the deflection of the kth tube, I_k and A_k are the moment of inertia and the cross-sectional area of the kth tube, the subscripts 1, 2,...N denote the quantities of the innermost tube, its adjacent tube, and the outermost tube, respectively, and all tubes have the same Young's modulus $E=1$ TPa and the mass density $\rho=1.3\ \mathrm{g/cm^3}$. Here, the ($N-1$) intertube interaction coefficients c_k ($k=1,2...N-1$) can be estimated using recent date given in Ref. 21 as

$$c_k=\frac{320\times(2R_k)\ \mathrm{ergs/cm^2}}{0.16d^2}, \quad d=0.142\ \mathrm{nm},$$

$$k=1,2...N-1, \qquad (2)$$

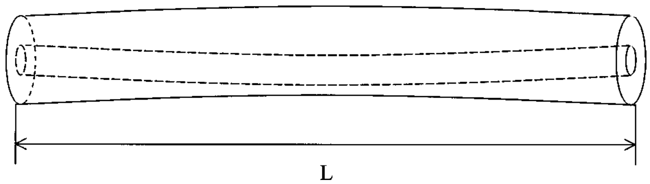

FIG. 1. Noncoaxial vibration of a doublewall carbon nanotube.

which are slightly larger than those used in Ref. 14.

Let us first consider a doublewall nanotube (DWNT) of length L, as shown in Fig. 1. Recently, the interest in DWNT's is rising due to the progress in large-scale synthesis of DWNT's.[21,22] Equations for a DWNT are given by the first two of Eq. (1) with $c_2=0$. Let us assume that all nested individual tubes have the same end conditions. Thus, it can be verified that all nested tubes have the same vibrational mode, $Y(x)$, determined by

$$d^4Y(x)/dx^4=\lambda^4Y(x) \tag{3}$$

with the given end conditions. The value λ and the mode $Y(x)$ are determined as the eigenvalue and eigenfunction of Eq. (3) under the given end conditions. For instance, for fixed end conditions, the first five eigenvalues of Eq. (3) are $\lambda_1L=4.73$, $\lambda_2L=7.85$, $\lambda_3L=10.9956$, $\lambda_4L=14.137$, and $\lambda_5L=17.278$. For cantilever end conditions, $\lambda_1L=1.875$, $\lambda_2L=4.694$, $\lambda_3L=7.855$, $\lambda_4L=10.996$, and $\lambda_5L=14.137$, see Ref. 23. Thus, for the n-order vibrational mode $Y_n(x)$ $(n=1,2...)$, the two n-order resonant frequencies of the DWNT can be obtained by substituting $w_1=a_1e^{i\omega t}Y_n(x)$, $w_2=a_2e^{i\omega t}Y_n(x)$ into Eq. (1), which yields

$$\omega_{n0}^2=\frac{1}{2}(\alpha_n-\sqrt{\alpha_n^2-4\beta_n}),\quad \omega_{n1}^2=\frac{1}{2}(\alpha_n+\sqrt{\alpha_n^2-4\beta_n}),$$

$$\alpha_n=\frac{EI_1\lambda_n^4+c_1}{\rho A_1}+\frac{EI_2\lambda_n^4+c_1}{\rho A_2}>\sqrt{4\beta_n},$$

$$\beta_n=\frac{EI_1EI_2\lambda_n^8}{\rho^2A_1A_2}+c_1\lambda_n^4\frac{EI_1+EI_2}{\rho^2A_1A_2}, \tag{4}$$

where the subscript 0 stands for the lowest (natural) n-order resonant frequency, in order to distinguish it from other $(N-1)$ n-order intertube resonant frequencies characterized by substantially noncoaxial vibrational modes. For each of the resonant frequencies, the associated amplitude ratio of vibrational modes of the inner to the outer tubes is

$$\frac{a_1}{a_2}=1+\frac{EI_2\lambda_n^4}{c_1}-\frac{\rho\omega^2A_2}{c_1}. \tag{5}$$

For the sake of comparison, the n-order resonant frequency of a MWNT given by the single-beam model[10–12] is

$$\omega_n^2=\lambda_n^4EI/(\rho A), \tag{6}$$

where I and A are the total moment of inertia and the total cross-sectional area of MWNT's. Thus, $I=I_1+I_2$ and $A=A_1+A_2$ for a DWNT. For a periodically supported MWNT, it is reasonable to assume that the deflection and the slope are zero at the supporters due to the symmetry. Thus, let us consider a fixed DWNT. For instance, assume that the inner and the outer diameters are 0.7 and 1.4 nm,

TABLE I. Resonant frequencies (10^{11} Hz) of a fixed DWNT (with the inner diameter 0.7 and the outer diameter 1.4 nm).

		Mode (n)				
	L/D_{out}	1	2	3	4	5
Natural frequency	10	14	38	72	106	141
	20	3.5	10	19	31	46
	50	0.6	1.6	3.1	5.1	7.5
Intertube frequency	10	103	107	123	162	225
	20	102	102	103	105	110
	50	102	102	102	102	102

TABLE II. Resonant frequencies (10^{11} Hz) of a cantilever DWNT (with the inner diameter 0.7 and the outer diameter 1.4 nm).

		Mode (n)				
	L/D_{out}	1	2	3	4	5
Natural frequency	10	2	14	38	72	106
	20	0.6	3.5	10	19	31
	50	0.1	0.6	1.6	3.1	5.1
Intertube frequency	10	102	103	107	123	162
	20	102	102	102	103	105
	50	102	102	102	102	102

TABLE III. Resonant frequencies (10^{11} Hz) of a fixed five-wall CNT (with the innermost diameter 0.7 and the outermost diameter 3.5 nm).

		Mode (n)				
	L/D_{out}	1	2	3	4	5
Natural frequency	10	4.9	13.4	25.5	38.9	50.5
	20	1.2	3.4	6.6	10.9	16.1
	50	0.2	0.5	1.1	1.8	2.6
Intertube frequency (ω_{n1})	10	53	54	57	65	80
	20	53	53	53	53	54
	50	53	53	53	53	53
Intertube frequency (ω_{n2})	10	90	91	93	97	106
	20	90	90	91	91	91
	50	90	90	90	90	90
Intertube frequency (ω_{n3})	10	122	122	123	127	133
	20	121	121	122	122	122
	50	121	121	121	121	121
Intertube frequency (ω_{n4})	10	145	145	147	150	157
	20	145	145	145	145	145
	50	145	145	145	145	145

respectively.[22] Thus, the two n-order resonant frequencies given by Eq. (4), for $n=1-5$, are listed in Table I for several smaller aspect ratios. It is found that (i) the natural frequency ω_{n0} given by Eq. (4) is close to that given by the single-beam model (6), with a relative error less than 1% for $n=1$, and less than 25% for $n=5$; (ii) the intertube resonant frequency ω_{n1}, about 10 THz, is insensitive to the mode number n, and is much higher than the lowest natural frequency ω_{10} for larger aspect ratios. Therefore, the single-beam model is accurate for coaxial vibrations of DWNT's of larger aspect ratios at relatively lower frequencies, such as those studied in Refs. 10–12; (iii) for shorter DWNT's, however, the lowest noncoaxial resonant frequencies are comparable to the first few higher natural frequencies. For example, for aspect ratio 10 (for which the beam model is adequate), the first few intertube frequencies ω_{n1} $(n=1-5)$ are around 10 THz, comparable to the third natural frequency $\omega_{30}=7.17$ THz and the fourth natural frequency $\omega_{40}=10.6$ THz. In this case, the noncoaxial intertube resonant frequencies and the associated noncoaxial vibrational modes will be excited at the higher natural frequencies.

Shorter cantilever MWNT's are used in some nanodevices (such as nanotweezers and AFM tips[7,8,24,25]). Here, the first few resonant frequencies of a shorter cantilever DWNT are listed in Table II. It is seen from Tables I and II that all conclusions obtained for fixed DWNT's remain qualitatively true for cantilever DWNT's. In particular, the lowest intertube resonant frequencies are almost the same in the two cases, indicating that they are insensitive to the end conditions. Additionally, for both fixed and cantilever DWNT's, the amplitude ratio a_1/a_2 of the inner to the outer tubes for the natural frequency ω_{n0} is always close to unity, indicating that the associated vibrational modes are almost coaxial. On the other hand, the amplitude ratio a_1/a_2 for the intertube resonant frequency ω_{n1} is about -0.7, indicating that the deflection of the inner tube is opposite to the deflection of the outer tube and thus the associated vibrational mode will distort otherwise concentric geometry of DWNT's. Since the concentric structure is the geometrical characteristic of MWNT's, such a noncoaxial intertube vibration would crucially affect some of their important physical properties.

Further, let us consider a five-wall CNT with the innermost diameter 0.7 and the outermost diameter $D_{\mathrm{out}}=3.5$ nm. In this case, for the n-order mode of Eq. (3) with the given end conditions, Eq. (1) gives five coupled equations which determine the n-order (lowest) natural frequency ω_{n0} and other four intertube resonant frequencies $\omega_{n1}<\omega_{n2}<\omega_{n3}<\omega_{n4}$. This phenomenon is similar to resonance of N coupled harmonic oscillators.[26,27] For example, for the fixed end conditions, all five resonant frequencies for $n=1-5$ are shown in Table III. It is seen that all results obtained for DWNT's remain qualitatively true for the five-wall CNT, while the lowest intertube resonant frequency now decreases to 5.25 THz. Again, it confirms that the single-beam model is relevant to coaxial vibrations of MWNT's of larger aspect ratios at relatively lower frequencies,[10–12] and noncoaxial vibrations occur only at much higher frequencies. Here, four noncoaxial intertube vibrational modes are shown in Fig. 2. It is seen that the intertube vibration causes complex

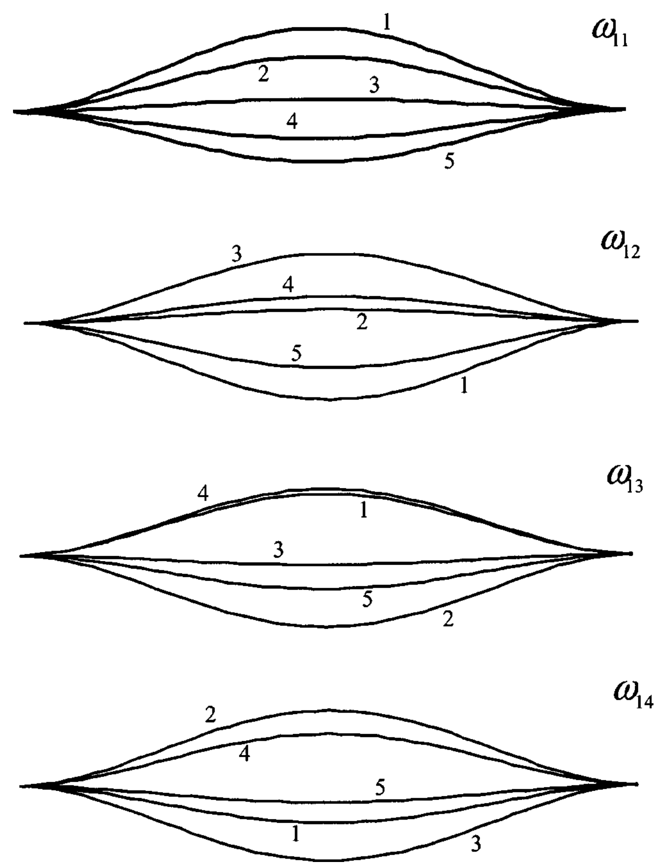

FIG. 2. Four noncoaxial intertube vibrational modes of a fixed five-wall CNT.

noncoaxial distortion of the MWNT. In particular, noncoaxial vibration could occur inside a MWNT even without significant deflection of the outermost tube. Of course, the jump of the deflections between any two adjacent tubes is bounded by the initial intertube spacing (about 0.34 nm). This is not a problem for small-deflection linear vibrations studied here.

In summary, different noncoaxial resonant frequencies and the associated noncoaxial vibrational modes are calculated. The first few noncoaxial resonant frequencies are found to be insensitive to vibrational modes, length of MWNT's, and the end conditions, while they decrease with the number of nested layers. For smaller aspect ratios, the lowest noncoaxial intertube resonant frequencies are found to be comparable to the first few higher (such as the third, fourth, or fifth) natural frequencies. This implies that internal noncoaxial resonance will be excited at the higher natural frequencies, and MWNT's cannot maintain their concentric structure at ultrahigh frequencies. In particular, because the first few intertube resonant frequencies fall into a very narrow range, their noncoaxial vibrational modes would be excited simultaneously. As a result, noncoaxial intertube vibration will distort otherwise concentric geometry of MWNT's, and thus crucially alter some of their important physical properties. Finally, it should be mentioned that the rapid advance in nanomechanical systems[28] is making it feasible or more practical to generate and detect vibrations in the terahertz range.[29,30]

[*]Corresponding author. Email address: c.ru@ualberta.ca

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