Frequency Study of Single-walled Carbon Nanotubes Based on a Space-frame Model with Flexible Connections

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***Abstract*—The dynamic behavior of the single-walled carbon nanotubes (SWCNTs) is studied based on the flexibly connected space-frame model which was proposed to simulate the static elastic properties of SWCNTs by the authors previously. The frequencies of SWCNTs with the clamped-free and clamped-clamped boundary conditions and the different ratios of length to diameter are computed. The resulting frequencies agree well with the solutions obtained from the sophisticated molecular dynamics models. In the predictions of equivalent moduli of SWCNTs, the flexibly connected space-frame model of carbon nanotubes yields a little bit lager moduli than the original space-frames model with rigid connections. In the present dynamics study, the flexibly connected space-frame model also gives the improved frequency prediction of SWCNTs than the original space-frame model. Consequently, the present vibration analysis shows that the flexibly connected space-frame model is a simple, efficient and accurate structural mechanics model to predict both the equivalent elastic moduli and the dynamic behaviors of carbon nanotubes.**

***Keywords*—carbon nanotubes; dynamic behavior; numerical simulations; equivalent structural mechanics model; flexibly connected space-frame.**

I. INTRODUCTION

Because of extremely unique physical structure and chemical structure, Carbon Nanotubes (CNTs) present some special mechanical, electrical, thermal, optical and chemical properties. Therefore, the CNTs have broad application prospect. In particular, as a new type of structural materials, CNTs have excellent mechanical properties, such as high modulus, high strength, high toughness, and low density. As a result, they can be widely used as an important component in MEMS/NEMS, ultrahigh frequency resonators as well as the reinforcements in various composite materials [1, 2]. The SWCNTs are small in size with large surface ratio and can respond to the external mechanical deformation rapidly with high sensitivity. The ultrahigh frequency of SWCNTs will facilitate the development of the fastest scanning probe microscopes, magnetic resonant force microscope, and even mechanical supercomputers. The predicted results of the elastic modulus of SWCNTs are widely accepted by most researchers, however, the predicted vibrating behaviors of SWCNTs given by different theories and models are considerably different. In view of this, it is desirable to present a simple and reliable dynamic analysis model in order to gain a complete understanding of dynamic behaviors of SWCNTs.

The method of experimental measurements is of high cost, and the measured results are very scattered. Though the method of the analytical analysis is relative cost-effective compared with the experimental method, it can only be applied in the cases of the CNTs with simple structures and subjected to simple deformations modes. As a result, the computer-based numerical methods are powerful tools to analyze the dynamics properties of carbon nanotubes with various loading and boundary conditions [1-3].

The numerical models can be grouped into the molecular dynamics model and the molecular mechanics/continuum mechanics model. The molecular structural mechanics model is one the simplest and most efficient models to simulate the static and dynamic behavior of CNTs among the various models proposed so far. Li and Chou [3] proposed an equivalent space-frame model with rigid connections to evaluate the elastic modulus and flexural frequencies of SWCNTs. However, the rigid connections can not correctly describe the bond angle change between the carbon atoms. On the basis of above analysis, a new equivalent flexibly connected space-frame model, named as the improved structural mechanics model in this paper, was proposed by the authors previous [4，5] and it is adopted in this work to analyze the vibration behavior of SWCNTs and to evaluate its accuracy in the vibration analysis of SWCNTs. The frequencies of SWCNTs with distinct chiralities, different boundary conditions and length-diameter ratios are evaluated in this paper. The resulting frequencies of SWCNTs agree well with the solutions given by the sophisticated molecular dynamic models and more accurate than those given by the space-frame model with rigid-connections [1]. Therefore, the flexibly connected space-frame model is simple, efficient and accurate structural mechanics model to evaluate both the equivalent elastic moduli and the dynamic behaviors of

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carbon nanotubes. The model presented in this paper has more potential applications in the mechanical analysis of carbon nanotubes and other nanomaterials.

II. Structual Mechanics Model Of CNTs

A. Theoretical Analysis

It is widely accepted that the response to foreign actions of the covalent bond between two neighboring carbon atoms can be simulated as an equivalent structural beam with a circular cross section [1]. The tensile stiffness *EA*, the flexural rigidity *EI* and the torsion stiffness *GJ* of the equivalent beam element can be determined based on the equivalence of the local potential energies in computational chemistry and the strain energy in structural mechanics [6]. As a result, the equivalent beam for the C-C bond of CNTs has the following mechanical properties:

$$\frac{EA}{L} = k_r, \quad \frac{EI}{L} = k_\theta, \quad \frac{GJ}{L} = k_\tau \tag{1}$$

where k_r, k_θ and k_τ are the force constants in molecular mechanics and L is the length of the equivalent beam. Then by using the method of structural mechanics, both the static and dynamic problems of CNTs can be solved numerically by using the finite element method.

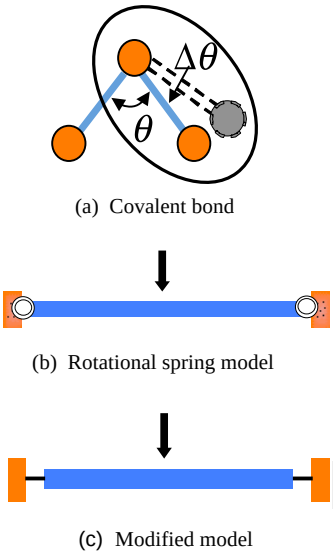
In order to determine the natural frequencies of SWCNTs, the condition of free vibration is considered in the equivalent space frame-like structure. For the problem of free vibrations of an undamped structure, the equation of motion is of the form:

$$[M]\{\ddot{q}\} + [K]\{q\} = \{0\} \tag{2}$$

Where $[M]$ and $[K]$ are the global mass matrix and stiffness matrix respectively, and $\{q\}$ and $\{\ddot{q}\}$ are the nodal displacement vector and acceleration vector. By taking the atomistic feature of a carbon nanotube into account, the masses of electrons are neglected and the mass of a carbon nuclei (m_c =1.993 × 10^{-26} kg) are assumed to be concentrated at the centers of atoms.

B. The Improved Structural Mechanics Model

The original structural mechanics model proposed by Li and Chou [1] is simple and efficient. The model is a space-frame structure with rigid connections depicted in Fig.2-1. Thus, the bond-angle changes under bending conditions shown in Fig.1a can not be described correctly in this original space-frame model. Shi *et al* proposed two models to characterize the behaviors of the nonlinear flexible connection in space-framed structures [7, 8]. Among these two models, the short beam model for the rotational spring illustrated in Fig.1b and Fig. 1c can be easily implemented with any existing finite element code. Based on the equivalent rotational spring model proposed by Shi *et al*. [7], an equivalent flexibly connected space-frame model, as illustrated in Fig. 2-2, was established for the predictions of the equivalent elastic properties of SWCNTs and the improved results were obtained by combining this improved structural mechanics model with the commercial finite element code, ANSYS [9].



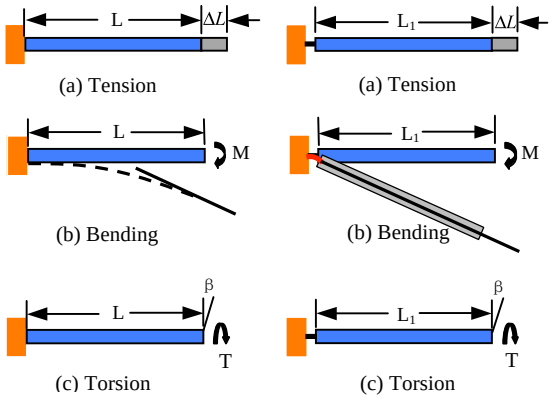
(a) Covalent bond

(b) Rotational spring model

(c) Modified model

Figure 1. Modeling of flexible connections

In the improved structural mechanics model, the short beam used between the nodes for the nuclei and the main beam for the C-C bond shown in Fig.2-2 has a normal stretching stiffness but a smaller bending stiffness [5]. These patterns of deformations in the equivalent beam are in good agreement with the real deformations of the covalent bond between carbon atoms. It can be seen from Fig.2 that the deformations under tension and torsion in the improved model are the same as the original space-frame model; however, the situation under the action of bending is totally different, i.e. the bond-angle change is allowed in the improved structural mechanics model.



(a) Tension (a) Tension

(b) Bending (b) Bending

(c) Torsion (c) Torsion

(1) a beam in original model (2) a beam in improved model

Figure 2. The deformations in the flexibly connected space-frame model

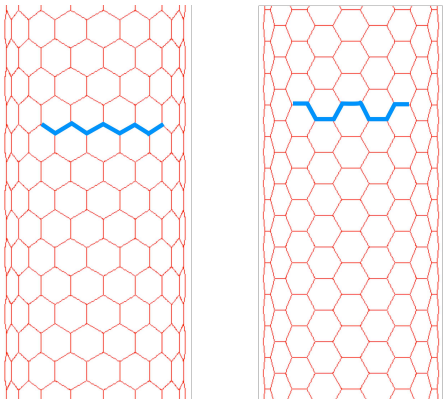
The lumped mass method, in which the masses of a structure are only concentrated at the nodes of the corresponding computational model, is used in the improved structural mechanics model. It was shown that the improved space-frame model is more accurate in

predicting the equivalent elastic properties of SWCNTs with distinct chiralities [4]. The performance of the improved space-frame model in the dynamic analysis will be studied in the next section.

III. COMPUTATIONAL MODEL OF CNTS

ANSYS [9] is used to establish the improved structural mechanics model and the Beam188 in ANSYS is chosen to be the beam element to build up the space-frame model. In this paper, the armchair and zigzag SWCNTs shown in Fig.3 are established and the force constants k_r,, k_θ and k_τ are given by:

$$\begin{cases} k_r = 6.52\times10^{-7}\, N/nm \\ k_\theta = 8.76\times10^{-10}\, N\cdot nm/rad^2 \\ k_\tau = 2.78\times10^{-10}\, N\cdot nm/rad^2 \end{cases} \quad (3)$$



(a) Zigzag (b) Armchair

Figure. 3. The equivalent structural model of CNTs

According to the force constants above, the tensile stiffness *EA*, the flexural rigidity *EI* and the torsion stiffness *GJ* can be determined easily as tabulated in Table 1 where the subscript 1 denotes the short beam element and the subscript 2 stands for the main beam element. The other relative parameters are also set according to the above analysis.

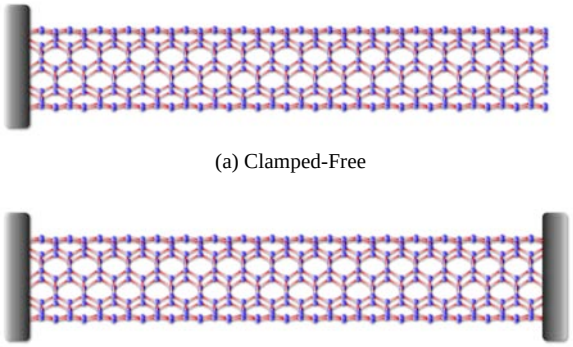
Table 1. The properties of beam elements for CNTs

Short beam	Main beam
L_1=0.0142 *nm*	L_2=0.1136 *nm*
EA_1=92.6343 *nN·nm*^{2}	EA_2= EA_1
EI_{y1}=EI_{z1}=0.0124 *nN·nm*^{4}	EI_{y2}=EI_{z2}=1000 EI_{y1}
GJ_1=0.0395 *nN·nm*^{2}	GJ_2= GJ_1

The length ratio of the short beam to the main beam is taken as 1:8 in the present study. The accuracy of this length ratio was verified with some properties simulations of SWCNTs. It was shown [4] that the resulting Young's modulus and shear modulus are in good agreement with the established results of the theoretical predictions and experimental evaluations. Therefore, the improved structural mechanics model with the selected length ratio of the short beam to the main beam is accurate in predicting the elastic properties of SWCNTs.

IV. VIBRATION ANALYSIS OF SWCNTS

The frequencies of nanotubes-based resonators depend on the tube chiralities, diameter, length as well as the boundary conditions of the nanotubes. In order to compare the results with those available in the open literature, two common chiralities of SWCNTs with different diameters, namely (5,5), (6,6), (6,0) and (8,0), and the two typical boundary conditions of the clamped-clamped and clamped-free SWCNTs depicted in Fig. 4 are considered in the present dynamic study.



(a) Clamped-Free

(b) Clamped-Clamped

Figure 4. The boundary conditions of carbon nanotubes

When the elastic properties given in Eq. (3) are substituted into the computational mode without the beam elements for the rotational springs, the same results as those in Ref. 1, which is based on the space-frame model with rigid connection proposed by Li and Chou [3], are obtained. However, when the beam properties given in Table 1 are applied to the present improved structural mechanics model shown in Fig.2-(2), the resulting flexural frequencies are larger than those given by Li and Chou [1] when the length to diameter ratio is less than 10, but they are closer to the results given by MD simulations [10, 11]. The fundamental frequencies of the SWCNTs as a function of the length to diameter ratio *L/D* given by the present improved space-frame model and those obtained from MD simulations [10, 11] as well the original structural mechanics model [1] under the two typical boundary conditions are plotted, respectively, in Fig 5. for the clamped-free condition and in Fig. 6 for the clamped-clamped conditions. It can be seen from the curves in the figures that the results obtained from the present flexibly connected space-frame model and the MD simulation are very close when the length to diameter ratio of SWCNTs is larger than 6. The relatively larger error in the present results with smaller SWCNTs aspect ratios of *L/D* is partially because the influences of the clamped boundary condition can not be neglected in the case of the tube are shorter (the length to diameter

ratio *L/D* is less than 6), and partially because the influences of the tube curvature on the out-of-plane bending stiffness is more profound for short tubes. Nevertheless, the capability and efficiency of the improved equivalent space-frame model have been verified in the predictions of the fundamental frequency of SWCNTs.

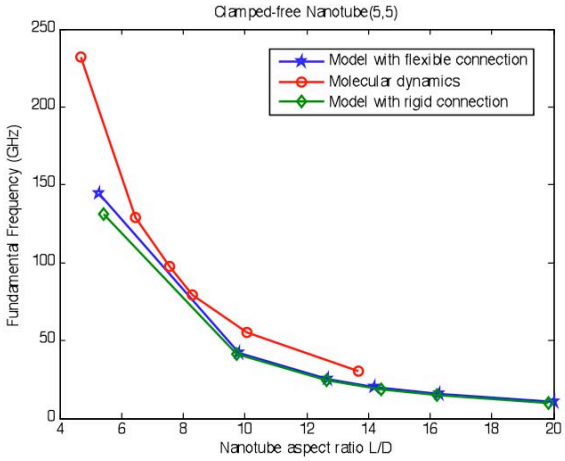


Figure 5. Fundamental frequencies of SWCNTs given by different methods (Clamped-Free)

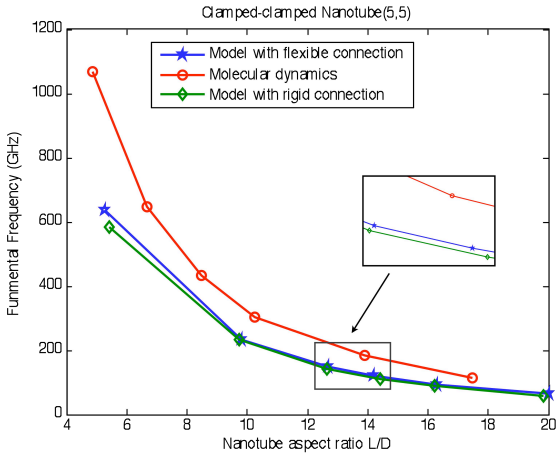


Figure 6. Fundamental frequencies of SWCNTs given by different methods.(Clamped-Clamped)

It is worthwhile to take a close look on the comparison between the present improved space-frame model and the original space-frame model. The frequency results of the SWCNTs as a function of the nanotube aspect ratio *L/D* given by the original rigidly connected space-frame model [1, 3] are also plotted in Fig. 5 and Fig. 6. It can be seen from the figures that the results predicted by both of these models are quite close each other when the ratio of the tube length to its diameter is larger than 10. However, the results given by the present space-frame model with flexible connections are better than those obtained from the original space-frame model with rigid connections in the case of shorter tubes.

The fundamental frequencies of SWCNTs with different chiralities and different diameters versus the length to diameter ratios are also studied. As shown in Fig. 7 and Fig. 8, the fundamental frequencies of SWCNTs decrease as the increase of the aspect ratios from 5 to 50. And the boundary conditions have significant influence on the fundamental frequencies.

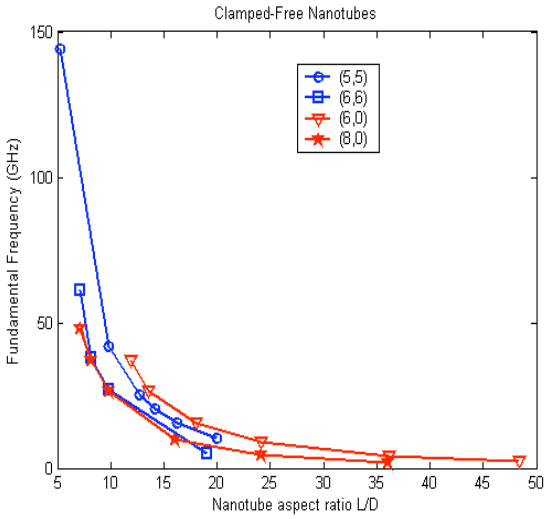


Figure 7. Fundamental frequencies of SWCNTs with different chiralities (Clamped-Free)

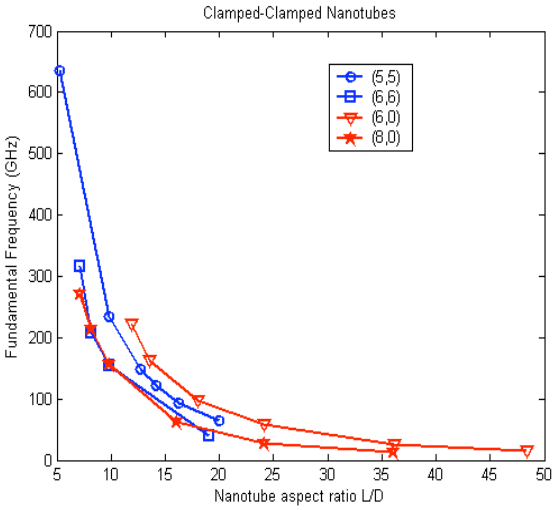


Figure 8. Fundamental frequencies of SWCNTs with different chiralities (Clamped-Clamped)

The variations of the fundamental frequencies as the function of the nanotube aspect ratios illustrated in Fig.7 and Fig.8 agree well with the solutions given by the MD simulations [10, 11]. And the tendency of the frequency variation with the diameter and aspect ratios of SWCNTs is also generally in accordance with the results reported in the literature [6, 10-12]. Consequently, the improved space-frame model with the flexible connections presented in this paper is an accurate and efficient model for the dynamic analysis of SWCNTs.

The higher vibration modes are also important in many applications of carbon nanotubes. The curves in Fig.9 and Fig.10 display the frequencies of the first ten vibration modes for different SWCNTs. For both types of boundary conditions, the frequencies of the first ten modes increase with the ranks of the vibration modes. And the chirality has an effect on the flexural frequencies of SWCNTs but not very significant.

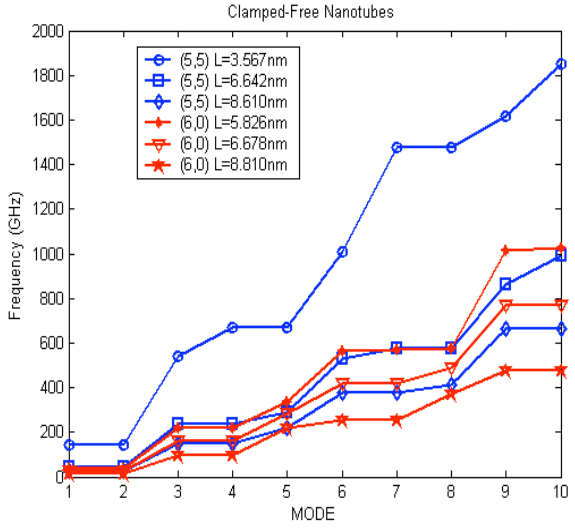


Figure 9. Frequencies of SWCNTs for the first ten modes (Clamped-Free)

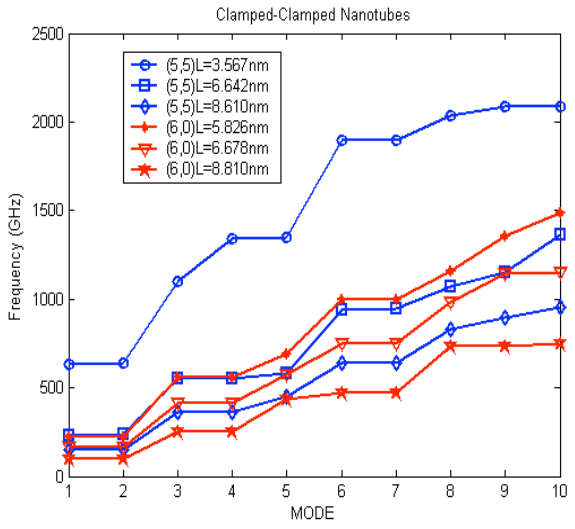


Figure 10. Frequencies of SWCNTs for the first ten modes. (Clamped-Clamped)

V. CONCLUSION

This paper presents the numerical study of the vibration behaviors of the clamped-clamped and clamped-free SWCNTs by using the flexibly connected space-frame model which is used to take account of the bond angle change of the SWCNTs. The analysis results given by the present improved structural mechanics model are in good agreement with the results obtained from the molecular dynamics models [11, 12] when the carbon nanotubes are long enough (the tube length to diameter ratio *L/D>6*), and the present flexibly connected space-frame model is more accurate than the original rigid space-frame model. Consequently, it can be concluded that the flexible connection model is a good approach to account for the C-C bond angle change in SWCNTs, and it is a necessary modification to the original structural mechanics model presented in Ref. 3.

The present flexibly connected space-frame model can be easily implemented in any commercial FEA codes and can be extended to the static and dynamic analysis of multi-walled nanotubes. Therefore, the present improved structural mechanics model is a simple, efficient and accurate structural mechanics model to simulate both the equivalent elastic moduli and the dynamic behaviors of carbon nanotubes.

ACKNOWLEDGMENT

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