

Resonant Frequency Analysis of Clamped-Free Multi-Walled Carbon Nanotube-Based Mass Sensor

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Abstract: In the present study, the vibrations of the clamped-free multi-walled carbon nanotube (MWCNT) with attached bacterium/virus on the free end have been investigated. To explore the suitability of the MWCNT as a bacterium/virus detector device, various viruses have been attached at free end to detect the resonant frequency of clamped-free MWCNT by using continuum mechanics approach. These results are compared with the analytical results, and it is found that the finite element method (FEM) simulation results are in good agreement with the analytical results. The results indicated the sensitivity and suitability of the MWCNT having different aspect ratio and different masses (attached at the free end of MWCNT) to identify the effects of bacterium or virus.

Keywords: Finite Element Model, Mass Sensors, Resonant Frequency, Sensitivity, Vibration

I. INTRODUCTION

Since their discovery in 1991, carbon nanotubes (CNTs) have generated huge activity in most areas of science and engineering owing to their unpredictable physical and chemical properties. No previous material has displayed the combination of superlative mechanical, thermal and electronic properties attributed to them.

Although discovered first, multi-walled carbon nanotubes (MWCNTs) [1] have not been studied as thoroughly as single-walled carbon nanotubes (SWCNTs). This could partly be due to the higher specific stiffness and strength of a SWCNT as compared to those of a MWNT. However, in certain applications, MWNTs offer superior properties over SWCNTs. For example, a MWNT is expected to have higher resistance to bending and buckling than a SWCNT. MWCNTs are easier to manufacture and are therefore less expensive than SWCNTs. They could conceivably be used as a bearing, as a pipe for transporting fluids. In the recent years it has been observed an explosion of interest in CNTs for applications in advanced electronics, biotechnology/medicine and sensors. In particular, studies have been performed for investigating mechanical behavior of CNT and the application of CNT as a bacterium/virus detector. I. Elishakoff [2] investigated the vibrations of the cantilever double-walled carbon nanotube (DWCNT) with attached bacterium on the tip in the view of developing the sensor. Chunyu Li [3] studied the promising application of carbon nanotubes as nano-resonators both single and double-walled carbon nanotubes are considered.

Resonance-based sensors offer the potential of meeting the high-performance requirement of many sensing applications, including metal deposition monitors, chemical reaction monitors, biomedical sensors, mass detector etc. [4], [5]. The merit of micromechanical resonators is that miniaturization of their dimensions enhances the mass sensitivity of these sensors [6]. If the resonators are scaled down to nanosize, the mass sensitivity of the resulting nano-sensors can surely be enhanced. The idea of using individual CNTs as high sensitivity nanobalances was first proposed [7]. Joshi et al. [8] suggested that the mass-sensing scale of CNT-based mass sensor can reach up to the Zeptogram level. Gupta et al. [9] has suggested that SWNTs are highly sensitive to mass which can be used in bio-medical field to detect various viruses having mass upto 10⁻⁶ of zeptogram.

Zhi-Bin Shen et al. [10] discussed the effects of the mass and position of the nanoparticle on the frequency shift in bridged single-walled carbon nanotube (SWCNT) carrying a nanoparticles.

Recent discoveries of various forms of carbon nanostructures have stimulated research on their applications in diverse fields. They hold promise for applications in medicine, drug and gene delivery areas. For instance, CNTs have the potential to carry drugs in the organism as they are hollow and much smaller than the blood cells. Detection of the mass of bio-molecules has become an increasing growing field in the biological and biomedical sciences.

Recently there has been a rapidly growing interest of CNTs in biological applications [11]–[14], in the field of medicine [15] and sensing mechanisms [16], [17] specifically as biosensors. The development of nano-biosensors [18] based on CNTs has been driven by the fact that biological objects such as proteins, enzymes and bacteria can be immobilized either in the hollow cavity or on the surface of CNTs. The methods were developed for attaching DNA and protein molecules to the inside and outside of the nanotube. This gives one the ability to target and destroy individual cells that may be cancerous or infected by a virus.

The principle of mass detection using nano-biosensors is based on the fact that the resonant frequency is very much sensitive to the mass of the bio-molecule, as with mass changes stiffness varies. The change of the attached mass on the CNT causes a shift to the resonant frequency. The key issue of mass detection is in quantifying the shift in the resonant frequency owing to the mass of the attached molecules.

II. BENDING VIBRATION OF A BEAM

Demetris Pentaras, Isaac Elishakoff [20] have shown that the free vibration of an MWCNT can be modeled by modifying the Bernoulli–Euler equation to include van der Waals interaction forces and solving N coupled equations for an N-walled CNT. Therefore, the governing differential equations for free vibration of the TWCNTs read

$$EI_1 \frac{\partial^4 y_1}{\partial x^4} + \rho A_1 \frac{\partial^2 y_1}{\partial t^2} = C_1 (y_2 - y_1) \quad (1)$$

$$EI_2 \frac{\partial^4 y_2}{\partial x^4} + \rho A_2 \frac{\partial^2 y_2}{\partial t^2} = C_2 (y_3 - y_2) - C_1 (y_2 - y_1) \quad (2)$$

$$EI_3 \frac{\partial^4 y_3}{\partial x^4} + \rho A_3 \frac{\partial^2 y_3}{\partial t^2} = -C_2 (y_3 - y_2) \quad (3)$$

Where E the Young's modulus, I_1, I_2 and I_3 are second moment of inertia, A_1, A_2 and A_3 are the cross-sectional area inner, intermediate and outer tube, $\rho = 2.3g/cm^3$ is the density of the beam material.

C_i is the van der Waals interaction coefficients for interaction pressure per unit axial length, which can be estimated based on an effective interaction width,

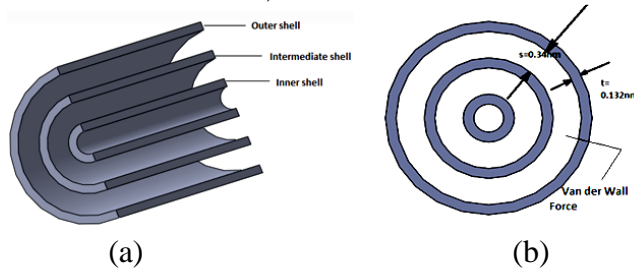


Fig.1. Continuum Model of MWCNT

$$C_i = 2R_i C_{12} \quad (4)$$

Where R_i is mean radius of each tube and C_{12} is the van derWaals interaction coefficients.

The van derWaals interaction coefficients C_{12} can be obtained through the Lennard – Jones pair potential

$$V(r) = 4\epsilon \left(\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right) \quad (5)$$

Where $\epsilon = 2.968 \times 10^{-3}$ eV, $\sigma = 0.3407$ nm and \bar{r} is the distance between two interacting atoms

From Eq. (A.9) [20], with van der Waals interaction taken into consideration, the dynamic equations for TWCNT becomes

$$\begin{bmatrix} K1 + K2 + C1 & -(K2 + C1) & 0 \\ -(K2 + C1) & K2 + K3 + C1 + C2 & -(K3 + C2) \\ 0 & -(K3 + C2) & K3 + C2 \end{bmatrix} \begin{bmatrix} y1 \\ y2 \\ y3 \end{bmatrix} - \omega_n^2 \begin{bmatrix} M1 & 0 & 0 \\ 0 & M2 & 0 \\ 0 & 0 & M3 \end{bmatrix} \begin{bmatrix} y1 \\ y2 \\ y3 \end{bmatrix} = 0 \quad (6)$$

Considering the value of the added mass as M , giving a virtual force at the location of the mass so that the deflection under the mass becomes unity, it can be shown that for a cantilevered CNT.

$$(K_{eq})_i = \frac{3EI_i}{L^3} \quad (7)$$

$$(M_{eq})_i = \frac{33}{140} \rho A_i L + m \quad (8)$$

where $i= 1, 2, 3$ and m is attached mass
 The resonant frequency can be obtained as

$$f_n = \frac{\omega_n}{2\pi} \quad (9)$$

Where ω_n is obtained by solving equation (6)

III. FINITE-ELEMENT APPROACH TO EQUIVALENT CONTINUUM MODELING

Using a hierarchical modeling scheme, the equivalent continuum modeling technique can be used to predict the bulk mechanical behavior of nano-structured materials. This study combines the continuum mechanics method with commercial FEM software to conduct the vibration analysis of a MWCNT approximated by a shell model with thickness and interlayer spacing. The resonant frequency of the MWCNT is simulated using a bending model.

In the present paper, MWNTs are treated as a number of concentric elastic cylindrical layers of SWNTs. Note that van der Waals force occur between any two neighbor atoms within effective distance; the simulation of this force is neglected in modeling a single nanotube since it is much smaller than molecular bond force. However, van der Waals force is the only interaction between layers when multi-layers problem is considered; its intrinsic nonlinearity and the construction of finite element mesh for any pairs of interactive atoms within the cutoff distance will need complicated and laborious modeling and computing effort. For simplification, it is proposed to employ Lennard-Jones model for interlayer pressure caused by van der Waals force instead of the force itself to be simulated. As CNT is assumed to be an isotropic material having mass density=2.3g/cm³, the Young's Modulus=2.54 TPa and the poisson ratio=0.23. Further, this study explores frequency change caused by various mass attached at free end as well as different position of cantilevered MWCNT.

IV. RESULT AND DISCUSSION

In present paper the finite element model of the MWCNT has been analyzed with the addition of different masses at free end as well as different position of cantilevered MWCNT. The model that has been developed for the purpose of analysis is shown in fig 3. The density and modulus of elasticity of MWCNT are taken to be 2.3 g/cm³ and 2.54 TPa, respectively. The mean radius of inner, intermediate and outer tubes are 0.246nm, 0.718 and 1.19 respectively, with different length of MWCNT (100nm, 150nm, 200nm and 250 nm) and the interlayer distance is 0.34nm with 0.132nm wall thickness. Fixed-free boundary condition has been taken for this analysis with variation in attached mass from 10-27 kg 10-21 kg for different lengths of MWCNTs. The position of attached mass has been varied from free end to fixed end of MWCNTs with mass of 10-18 kg. Fig 2 represents different mode of vibration of MWCNT with mass attached at its free end.

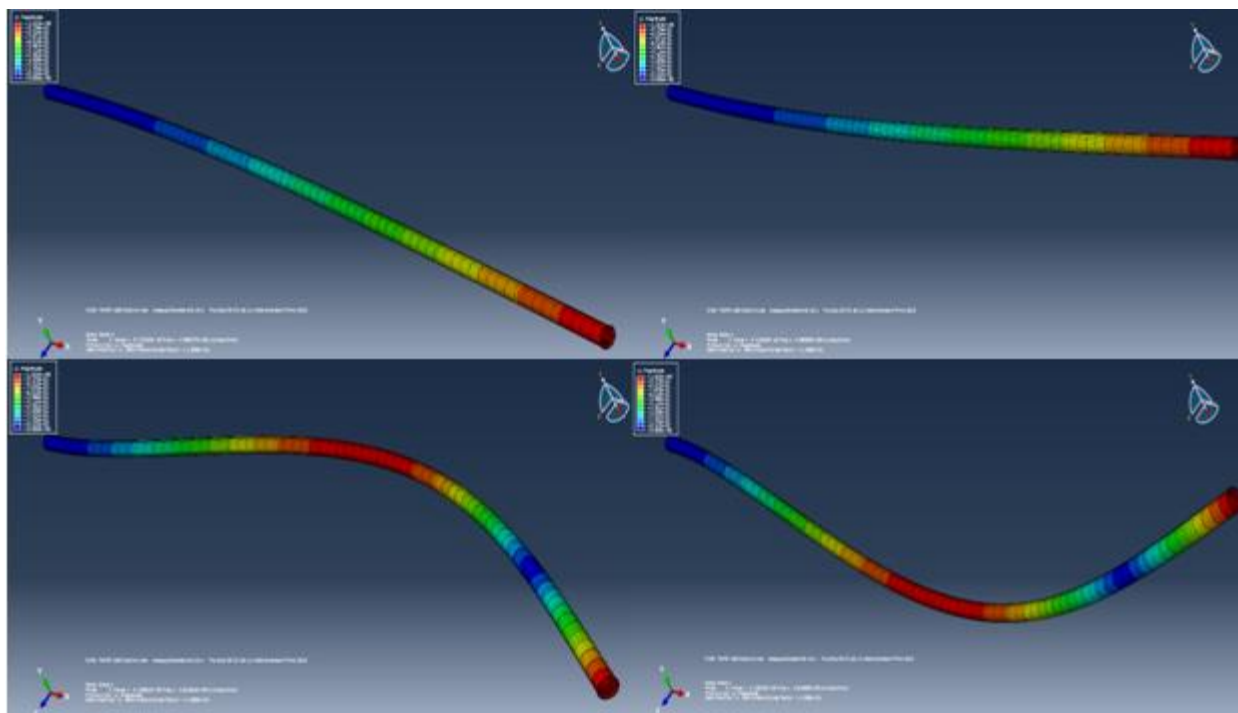


Fig.2. Different Mode Shapes

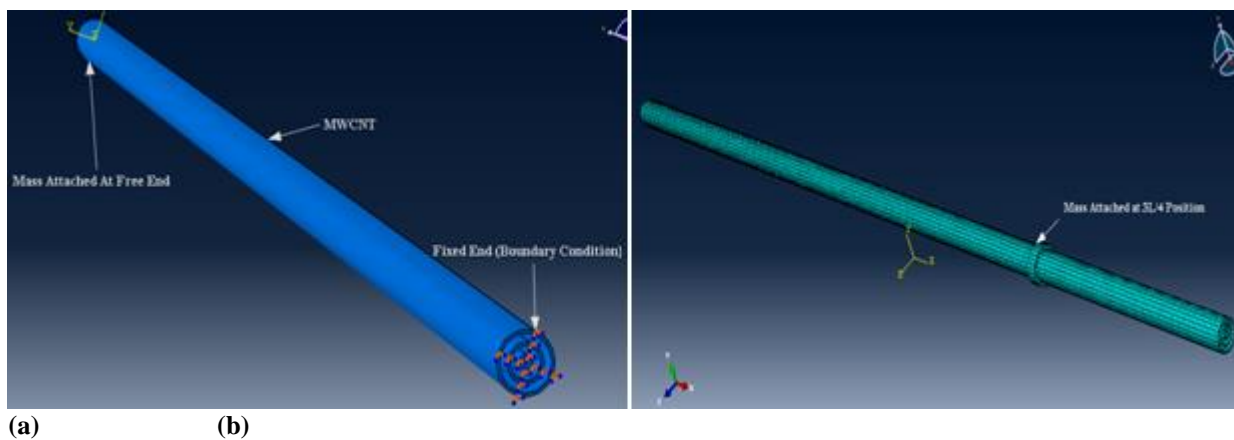


Fig.3. Enlarged view of FE model of MWCNT

TABLE I: Resonant frequency (GHz) with masses attached at tip of Clamped-free MWCNT for different length.

Attached Mass(kg)	L=100nm		L=150nm		L=200nm		L=250nm	
	FEM	Analytical	FEM	Analytical	FEM	Analytical	FEM	Analytical
10^{-20}	0.08	0.082	0.041	0.045	0.021	0.02949	0.014	0.0214
10^{-21}	0.22	0.28	0.117	0.138	0.081	0.09	0.058	0.0648
10^{-22}	0.58	0.7	0.296	0.356	0.197	0.219	0.131	0.158
10^{-23}	0.98	1.18	0.485	0.549	0.275	0.319	0.176	0.21
10^{-24}	1.22	1.32	0.554	0.595	0.307	0.34	0.202	0.221
10^{-25}	1.29	1.34	0.574	0.602	0.327	0.3422	0.217	0.222
10^{-26}	1.3	1.34	0.575	0.603	0.327	0.3422	0.217	0.222
10^{-27}	1.3	1.34	0.575	0.603	0.327	0.3422	0.217	0.222

TABLE II: Frequency shift with variation in magnitude of the mass

Attached Mass(kg)	Frequency Shift (GHz)			
	L=100nm	L=150nm	L=200nm	L=250nm
10^{-20}	1.22	0.534	0.306	0.203
10^{-21}	1.08	0.458	0.245	0.159
10^{-22}	0.72	0.279	0.13	0.086
10^{-23}	0.32	0.09	0.052	0.041
10^{-24}	0.08	0.021	0.02	0.015
10^{-25}	0.01	0.001	0	0

Table I summarizes the various masses that have been taken for analysis along with their mass. The FEM solution and the analytical results have been compared for the first resonant frequency for different attached masses and different length for clamped-free boundary condition of MWCNTs. The comparative results between the analytical and FEM-simulated results confirm the validity of the current FE model and indicate its suitability for use in the further investigation of the MWCNT as a mass sensor.

Table II summarizes the variation in frequency shift due to change in magnitude of attached masses for different length of CNTs

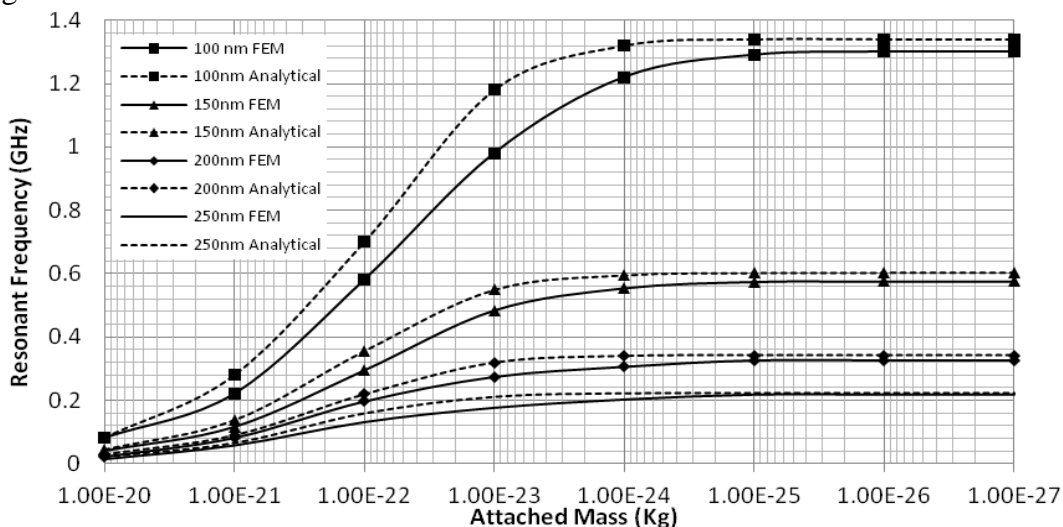


Fig. 4. Variation of resonant frequency with different attached mass for different length of MWCNT

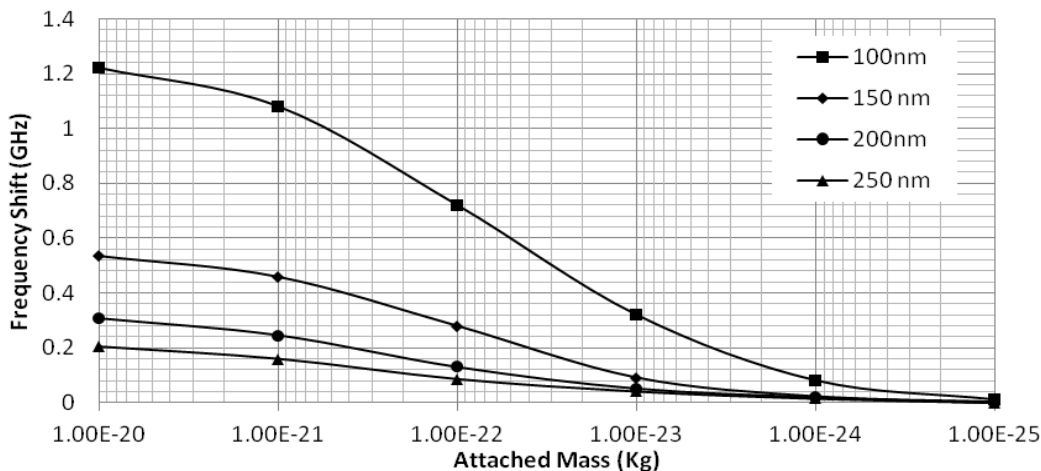


Fig.5. Variation of frequency shift with different attached mass for different length of MWCNT

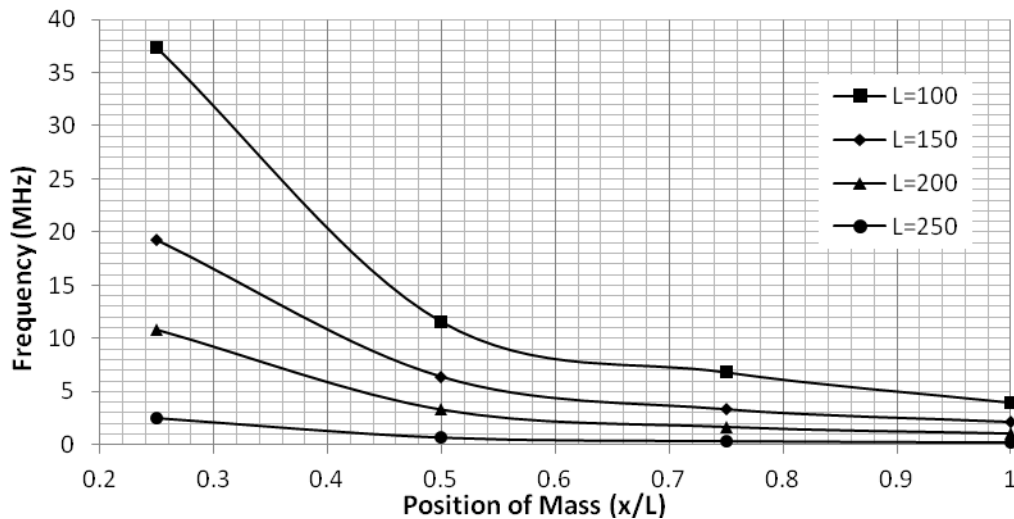


Fig.6. Frequency variation with position of mass at MWCNT

Fig. 4 compares the resonant frequencies obtained by FEM simulation and analytical solution for various lengths of MWCNT and attached masses. Trend of variation followed by resonant frequencies is same for both FEM simulation and analytical solution. It is shown that the FEM simulation results are in good agreement with the analytical data. Change in frequency is noticeable upto 10-25kg, beyond this there is no clear change in resonant frequencies.

It is observed that resonant frequency increases with decrease in attached mass. It is also observed that resonant frequency decreases as length of MWCNT increases. For 100nm long MWCNT, frequency shift is large, but as the length increases frequency shift goes on decreasing as shown in fig.5.

From fig.6 it is also observed that as the attached mass moves from fixed end and approaches towards free end, the resonant frequency decreases. For shorter length frequency change is higher as compared to longer CNTs.

V CONCLUSION

1. The present work has analyzed the modeling of MWCNTs using a Finite Element Model.
2. This analysis explores the resonant frequencies of MWCNTs caused by changes in size of CNT in terms of length, changes in magnitude and position of attached masses.
3. The mass sensitivity of carbon nanotube based mass sensor is different for different length of CNTs, magnitude and position of attached masses as shown in fig. 4 & 6. It is clear from the figure that when length of MWCNTs increases the resonant frequency decreases.
4. It is also observed from the fig. 4, with increase in magnitude of attached mass there is corresponding decrease in resonant frequency and sensitivity of MWCNT based mass sensors reaches upto 10-25kg.
5. Also it is clear from fig. 6 that as mass approaches towards fixed end of MWCNT there is increase in resonant frequency. Hence for better sensitivity it is obvious to attach mass at tip of the clamped-free MWCNTs where frequency shift is higher as explored in fig. 5.

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