Vibration Analysis Of Clamped-Free Multi-Walled Carbon Nanotube-Based Bio-Sensors Because Of Various Viruses

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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.

“1. 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 SWNT as compared to those of a MWNT. However, in certain applications, MWNTs offer superior properties over SWNTs. 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 behaviour 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 by Poncharal et al. [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.

“2.Basic theoretical analysis”

Recently, the continuum mechanics method has been successfully applied to analyze the dynamic responses of individual CNTs.

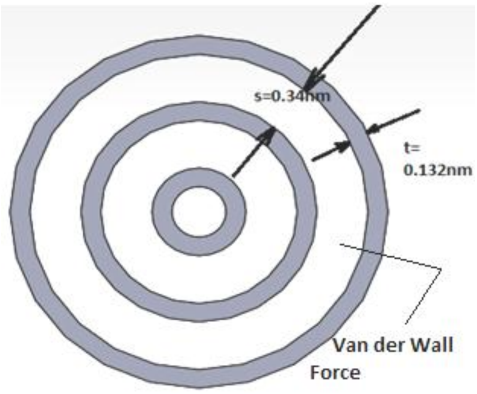
“2.1 Bending vibrations of a beam”

Demetris Pentaras, Isaac Elishakoff [19] have shown that the free vibration of an MWCNT can be modelled 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

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

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

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



“Fig. 1. Continuum model of MWCNT”

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, $\rho=2.3g/\mathrm{cm}^3$ is the density of the beam material. [20] 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 [He et al. (2005)]

$$C_i=2R_iC_{12} \qquad (4)$$

Where R_i is mean radius of each tube and C_{12} is the van der Waals interaction coefficients.
The van der Waals interaction coefficients C_{12} can be obtained through the Lennard–Jones pair potential [Jones (1924)],

$$V(r)=4\varepsilon\left(\left(\frac{\sigma}{\bar{r}}\right)^{12}-\left(\frac{\sigma}{\bar{r}}\right)^{6}\right) \qquad (5)$$

Where $\varepsilon = 2.968 \times 10^{-3}$ 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

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

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

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

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

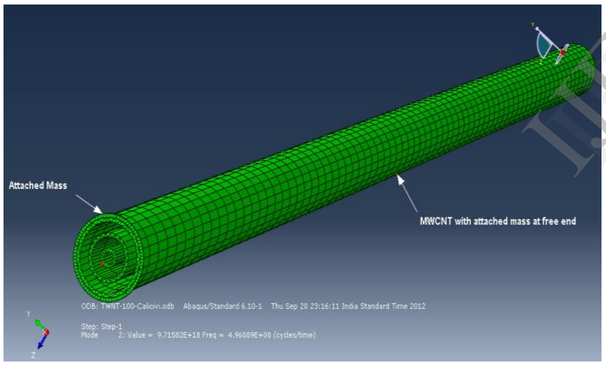
Where i = 1, 2, 3 and m is attached mass
The resonant frequency can be obtained as

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

Where ω_n is obtained by solving equation (6)

"3. Finite-element approach to equivalent continuum modeling"

Using a hierarchical modeling scheme, the equivalent continuum modeling technique [21, 22] 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 shown in figure 2.

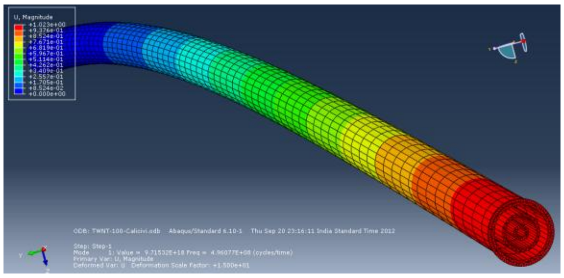


"Fig.2. Enlarged view of FE model of MWNT"

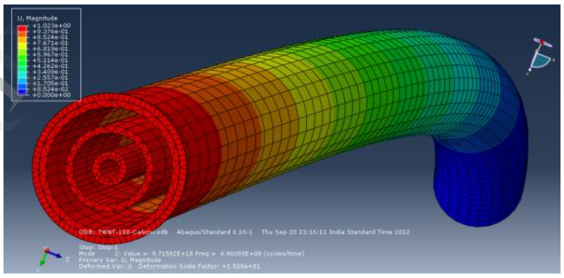
In the present paper, MWNTs are treated as a number of concentric elastic cylindrical layers of SWNTs. Note that van der Waals force occurs between any two neighbour atoms within effective distance; the simulation of this force is neglected in modelling a single nanotube since it is much smaller than 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 modelling and computing effort. For simplification, it is proposed to employ Lenard-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/cm^3, the Young's Modulus=2.54 TPa and the poison ratio=0.23. Further, this study explores frequency change caused by the bacterium/virus attached at the tip of cantilevered MWCNT.

"4. Result and discussion"

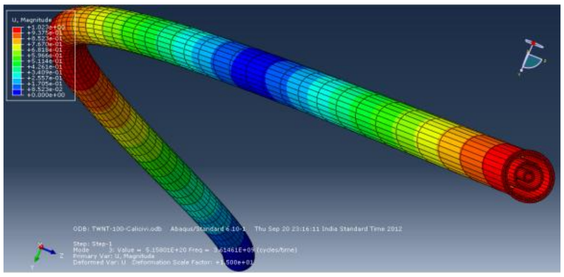
First five mode shapes are shown as below:



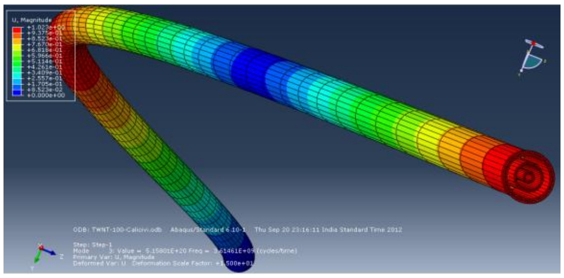
"Fig. 3 First Mode"



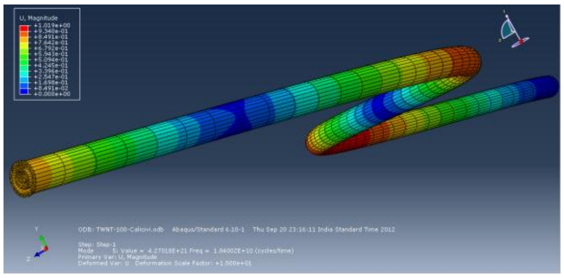
"Fig. 4 Second Mode"



"Fig. 5 Third Mode"



"Fig.6. Fourth Mode"



“**Fig. 7** Fifth Mode”

A clamped-free MWCNT is used for simulating its behaviour owing to the attached bacterium/virus at the tip. The density and modulus of elasticity of MWCNT are taken to be 2.3 g/cm^3 and 2.54 TPa, respectively.
The mean radius of inner, intermediate and outer tubes is 0.246nm, 0.718 and 1.19 respectively, with different aspect ratios (20, 40, 60, 80 and 100) and the interlayer distance is 0.34nm with 0.132nm wall thickness.
The mass of the MWCNT is 4.099X10^{-22} kg. When an atom or molecule is deposited onto the CNT, the tube’s resonant frequency changes in proportion to the mass of the atom or molecule attached. Measuring this change in frequency reveals the mass of the impinging atom or molecule.
Table 1 summarizes the various bacterium/viruses 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 mass and different aspect ratios 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 that can be used as a bacterium/virus detector.

“**Table 1.** Resonant frequency of MWCNT with attached bacterium/viruses at the tip of CNT for different aspect ratio of CNT (L/D)”

Virus/Becterium	Mass (kg)	Resonant frequency(Hz)									
		L/D=20		L/D=40		L/D=60		L/D=80		L/D=100	
		Analytical	FEM	Analytical	FEM	Analytical	FEM	Analytical	FEM	Analytical	FEM
Parvoviridae Largest	1.29E-20	2.05E+08	2.09E+08	7.26E+07	7.79E+07	3.96E+07	4.02E+07	2.60E+07	2.67E+07	1.89E+07	2.17E+07
Parvoviridae Smallest	4.28E-21	3.60E+08	3.82E+08	1.25E+08	1.28E+08	6.90E+07	6.59E+07	4.48E+07	4.55E+07	3.26E+07	3.70E+07
Orthomyxoviridae	6.23E-22	9.80E+08	1.05E+09	3.20E+08	3.30E+08	1.72E+08	1.91E+08	1.11E+08	1.07E+08	8.00E+07	8.68E+07
Togoviridae Smallest	2.25E-22	1.48E+09	1.62E+09	5.06E+08	5.67E+08	2.66E+08	3.08E+08	1.69E+08	1.51E+08	1.19E+08	1.40E+08
Polyoma	6.30E-23	2.55E+09	2.68E+09	8.11E+08	8.46E+08	4.05E+08	4.03E+08	2.48E+08	2.21E+08	1.70E+08	1.79E+08
Staphilococcus	5.60E-23	2.66E+09	2.75E+09	8.40E+08	8.54E+08	4.20E+08	4.11E+08	2.55E+08	2.31E+08	1.74E+08	1.84E+08
Togoviridae Largest	4.19E-23	2.99E+09	3.10E+09	9.10E+08	9.13E+08	4.47E+08	4.29E+08	2.70E+08	2.43E+08	1.83E+08	1.87E+08
Caliciviridae	3.94E-23	3.02E+09	3.20E+09	9.20E+08	9.36E+08	4.55E+08	4.39E+08	2.73E+08	2.49E+08	1.84E+08	1.91E+08
Nudaurelia	2.90E-23	3.34E+09	3.51E+09	9.98E+08	1.01E+09	4.82E+08	4.62E+08	2.87E+08	2.59E+08	1.92E+08	1.98E+08

Table 2 shows the variation in the frequency shift for different aspect ratio of CNT. It is clear from the table that as the length of CNT decreases frequency shift increases subsequently. Hence it can be concluded that for shorter length CNT becomes more sensitive when the mass is attached at the tip.

Table 3 shows the percentage error in FEM-simulated frequency. It is evident from the table that FEM-simulated result has close proximity with the exact solution. The percentage error varies from 0.295 to 15.1, which is quite acceptable. Hence, the model developed in this paper can be used for further investigation.

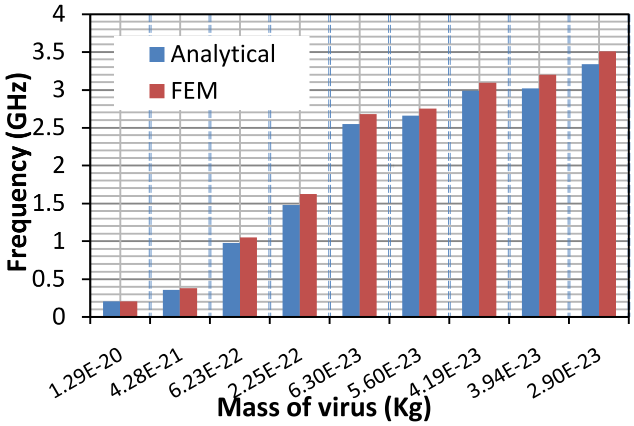
“**Table 2.** Percentage frequency shift”

Virus/Becterium	Mass (kg)	% Resonant frequency shift				
		L/D=20	L/D=40	L/D=60	L/D=80	L/D=100
Parvoviridae Largest	1.29E-20	95.89406	93.42514	91.91894	90.5	89.8
Parvoviridae Smallest	4.28E-21	92.48956	89.20259	86.75431	83.8	82.61855
Orthomyxoviridae	6.23E-22	79.31265	72.16988	61.68303	61.8	59.21418
Togoviridae Smallest	2.25E-22	68.06687	52.18731	38.04532	46.3	34.11501
Polyoma	6.30E-23	47.27367	28.62012	18.95618	21.2	15.79347
Staphilococcus	5.60E-23	45.87391	27.92138	17.52192	17.7	13.50215
Togoviridae Largest	4.19E-23	39.1104	23.00964	10.34872	13.4	11.99261
Caliciviridae	3.94E-23	37.10048	21.03745	11.77271	11.2	10.02
Nudaurelia	2.90E-23	31.03637	14.70006	7.145879	7.70	6.730382

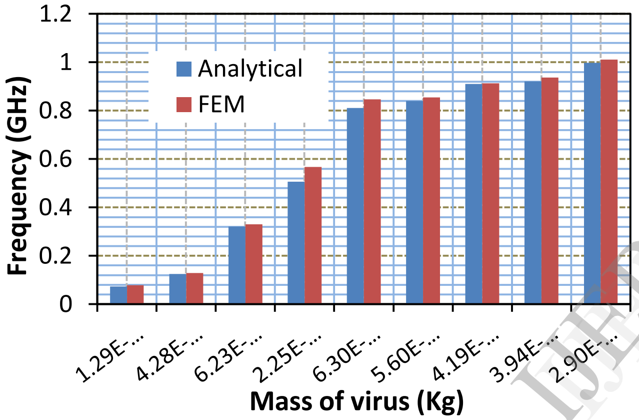
“**Table 3.** Percentage error in the FEM-simulated frequency”

Virus/Becterium	Mass (kg)	% Error in resonant frequency				
		L/D=20	L/D=40	L/D=60	L/D=80	L/D=100
Parvoviridae Largest	1.29E-20	1.86	7.36	1.55	2.56	13
Parvoviridae Smallest	4.28E-21	5.78	2.34	4.44	1.55	11.8
Orthomyxoviridae	6.23E-22	6.89	3.01	9.82	3.41	7.80
Togoviridae Smallest	2.25E-22	8.90	10.7	13.7	10.8	15.1
Polyoma	6.30E-23	4.94	4.16	0.392	10.8	5.10
Staphilococcus	5.60E-23	3.40	1.69	2.25	9.42	5.44
Togoviridae Largest	4.19E-23	3.48	0.295	3.97	9.97	2.26
Caliciviridae	3.94E-23	5.63	1.72	3.48	8.72	3.88
Nudaurelia	2.90E-23	4.80	1.31	4.11	9.72	3.35

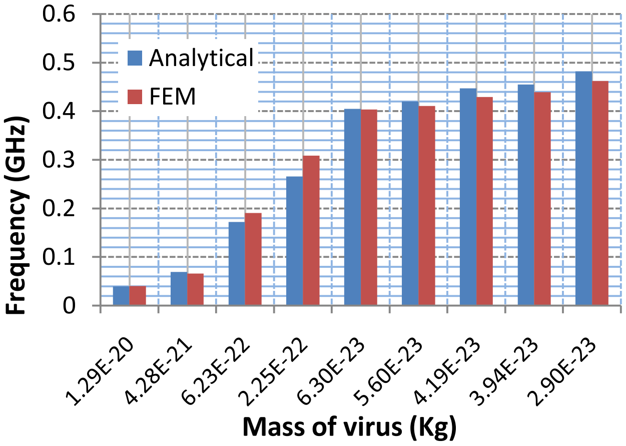
Figs.(7-12) show the comparison between the analytical results and the FEM solution for the different aspect ratio of MWCNT when the different bacterium/virus is attached at the tip. Fig.(13) represent variation of %age frequency shift for mass of various viruses attached at the tip of tube. It is evident from the figures that the FEM results are in the closed proximity with the analytical results. Through the figures, it is evident that by reducing the length of the MWCNT, the improvement of the sensitivity of the sensor can be possible.



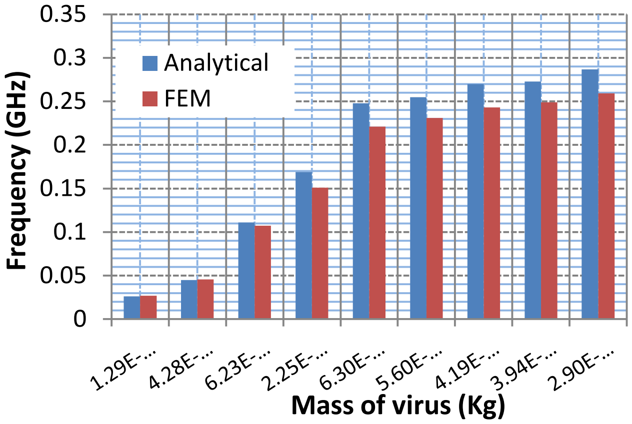
“**Fig. 8** Frequency vs. mass with attached virus/bacterium at the tip for L/D=20”



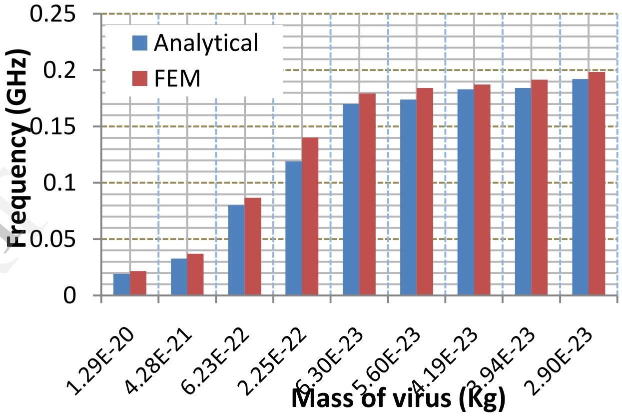
“**Fig. 9** Frequency vs. mass with attached virus/bacterium at the tip for L/D=40”



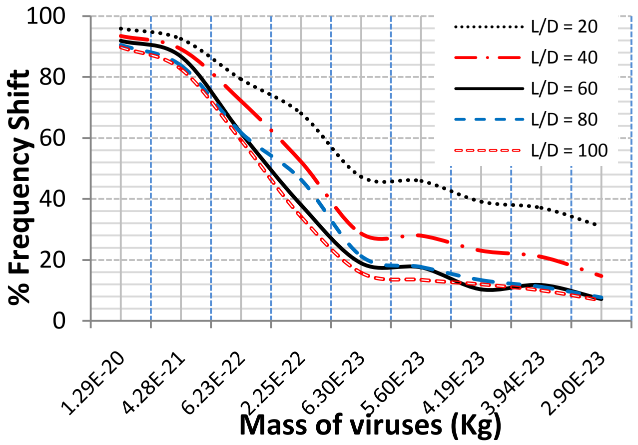
“**Fig. 10** Frequency vs. mass with attached virus/bacterium at the tip for L/D=60”



“**Fig. 11** Frequency vs. mass with attached virus/bacterium at the tip for L/D=80”



“**Fig. 12** Frequency vs. mass with attached virus/bacterium at the tip for L/D=100”



“**Fig. 13** Percentage frequency shift vs. mass of attached virus/bacterium at the tip for various aspect ratio”

“5. Conclusion”

Vibration of a cantilever MWCNT with attached various masses of virus at the tip have been studied in this paper. Several bacteria or virus masses have been chosen (as shown in Table 1) and feasibility of CNT as a bacterium/ virus detector has been shown. CNTs are the most promising materials for this purpose and their small size makes them sensitive enough to resolve single atoms even at room temperature. Although scientists already have the ability to measure the mass of individual atoms through a complex technique known as mass spectrometry this new CNT-based mass sensor offers some distinct advantages like it does not require the ionization of neutral atoms or molecules that can destroy samples such as proteins while sensing the mass. CNT is small enough so that it could be incorporated onto a chip in future.

It is concluded that frequency shift increases subsequently due to decrease in length of CNT. Hence it is obvious that shorter length CNT becomes more sensitive when the mass is attached at the tip. Finally it can also be concluded that deposition of an atom or molecule onto the CNT, the tube’s resonant frequency changes in proportion to the mass of the atom or molecule attached.

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