Vibrational properties of carbon nanotube (CNT)

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Abstract: The present article is concentrated to study the vibrational properties of carbon nanotube through weak interaction method specially single walled carbon nanotube. SWNT acts as pure quntum elements in which electrons move in axial direction of the tube and it may decompose at temperature higher than 550℃. It is theoretically ensured that frequency of vibration of carbon nanotube tends to increase as the tube diameter decreases so as to resonant frequency set up in easier way. Originally vibrational frequency of carbon nanotube depends on chiral vector C and nanotube diameter d_t. virtual calculation has been done to show the dependence of frequency on nanotube diameter in different order of atomicity (m, n). The length of nanotube is not arbitrarily rather with respect to nanotube diameter as if volume maintaining constant. The theoretical data have also been compared to Donnel thin shell theory where model deformation displacement are interpretated.

Key words: Vibrational frequency. Weak interaction method, single wall nanotube, resonant frequency, Thin shell model.

I INTRODUCTION

Carbon nanotube is the thinnest material [1] ever increasing in the world based on rolled-up grapheme layers [2]. It has unique and remarkable properties to fascinate the world. Vibrational properties of CNTs and their corresponding applications in different areas are known to all in our science- technology such as electronic, optical, medicine, charge detectors, sensors, field emission devices, aerospace, defence construction and even fashion[1]. The vibration of CNTs have been studied extensively in the last two decades and various effective models such as thin shell model[3], beam, ring as well as other continuum models[4]. It is even now more exploration to investigate the vibrational characteristics of CNTs, SWNT have significant role in material strength and in practical too. A reliable knowledge of vibrational data is significant for optimized design of process and apparatus in various engineering and science fields. New innovative improvement and technologies are to be executed such as nano-probes, emanation, panel spectacle, nano-electronics, chemical sensing and drug deliverance.

The vibration of SWNTs can be investigated experimentally, theoretically and by simulation techniques. This paper is based on some aspects be regarded as an update of earlier reviews on different numerical simulations to compute the frequency of SWNTs. The frequency of vibration is virtually calculated and compared to thin shell model. Weak interaction method is an appropriate to determine the frequency of vibration of carbon nanotube ascertains vibratinal characteristics.

II THEORY AND TECHNIQUE

The vibrational property of carbon nanotube depends on the ratio of chiral vector c and nanotube diameter d_t i.e. vibrational frequency,

$$\omega = \frac{C}{d_t} \qquad \ldots\ldots\ldots\ldots\ldots \qquad \ldots\ldots\ldots\ldots\ldots(1)$$

If we consider chiral vector c as constant, the frequency depends on nanotube diameter, d_t. At constant temperature, electrons move in axial direction of the tube and it decomposes at temperature higher than 550℃. The current due to axial movement of electrons consists of

$$I = \frac{q}{t}$$

$$I = \frac{ne}{t} \quad \ldots\ldots \qquad ..(2)$$

If electrons move with Fermi velocity, $v_f = \frac{l}{t}$

Where, l = length of the tube, from eq.(2)

$$I = \frac{ne}{l/v_f}$$

$$I = \frac{nev_f}{l} \qquad \ldots(3)$$

It is clear that current is directly proportional to Fermi velocity in carbon nanotube.

Now according to Donnel thin shell theory, if u,v and ω are longitudinal circumferential and radial displacement of the shell, R is the radius of the shell Eh = in-plane rigidity, ρh = mass density per unit lateral area, v =Poisson's ratio.

Model deformation displacement are given by [5, 7]

U(x, θ, t) = $a_m.e^{-i(k_m x-\omega t)}$.sin$\theta$ ………(4)

V(x, θ, t) = $b_m.e^{-i(k_m x-\omega t)}$.cos$\theta$ ……..…(5)

ω(x, θ, t) = $c_m.e^{-i(k_m x-\omega t)}$.sin$\theta$ …..……(6)

Where a_m, b_m, and c_m are vibrational amplitude coefficients.

Here, (m, n) axial half and circumferential wave number, f = $\frac{\omega}{2\pi}$

k_m = axial wave number

The three unknown displacement functions are given by.

$$\frac{\partial^2 u}{\partial x^2}+\frac{1-v}{2R^2}.\frac{\partial^2 u}{\partial \theta^2}+\frac{1+v}{2R}.\frac{\partial v}{\partial x.\partial \theta}-\frac{v}{R}.\frac{\partial \omega}{\partial x}=(1-v^2).\frac{\rho h}{Eh}.\frac{\partial^2 u}{\partial t^2}. \quad (7)$$

$$\frac{1+v}{2R}.\frac{\partial^2 u}{\partial x.\partial \theta}+\frac{1-v}{2}.\frac{\partial^2 v}{\partial x^2}++\frac{1}{R^2}.\frac{\partial^2 v}{\partial \theta^2}-\frac{1}{R^2}.\frac{\partial \omega}{\partial \theta}=(1-v^2).\frac{\rho h}{Eh}.\frac{\partial^2 v}{\partial t^2} \quad (8)$$

$$\frac{v}{R}.\frac{\partial u}{\partial x}+\frac{1}{R^2}.\frac{\partial v}{\partial \theta}-\left(\frac{1}{R^2}+\frac{1-v^2}{Eh}\right)\text{D}.\left(\frac{\partial^4 \omega}{\partial x^4}+2\frac{1}{R}\frac{\partial^4 \omega}{\partial x^2 \partial \theta^2}+\frac{1}{R^4}.\frac{\partial^4 \omega}{\partial \theta^2}\right)=(1-v^2).\frac{\rho h}{Eh}.\frac{\partial^2 u}{\partial t^2}\ldots \quad (9)$$

Where, D = $\frac{Eh^3}{12(1-v^2)}$ = effective bending stiffness.

Now the simplified form is reduced to

$$\left(k_m^2+\frac{1-v}{2R^2}.n^2\right).a_m+\left(ik_m.\frac{1+v}{2R}.n\right)b_n+(ik_m.\frac{v}{R})c_m=(1-v^2).\frac{\rho h}{Eh}.\omega_{a_m}^2. \quad (10)$$

$$\left(-n.ik_m.\frac{1+v}{2R}\right)a_m+\left(\frac{1-v}{2}k_m^2+\frac{1}{R^2}.n^2\right)b_m+\frac{n}{R^2}c_m=(1-v^2).\frac{\rho h}{Eh}.\omega_{b_m}^2.(11)$$

$$\left(-\frac{v}{R}.ik_m\right)a_m+\frac{n}{R^2}b_m+-\left(\frac{1}{R^2}+\frac{1-v^2}{Eh}D.(k_m^4+\frac{2}{R^2}k_m^2.n^2+\frac{n^4}{R^4}\right)c_m==(1-v^2)\frac{\omega^2}{Eh}\ \ldots\ldots(12)$$

In matrix form these equations are written as

$$\begin{pmatrix}A_{11} & A_{12} & A_{13}\\ A_{21} & A_{22} & A_{23}\\ A_{31} & A_{32} & A_{33}\end{pmatrix}\begin{pmatrix}a_m\\ b_m\\ c_m\end{pmatrix}=(1-v^2)\frac{\omega^2\rho h}{Eh}\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\begin{pmatrix}a_m\\ b_m\\ c_m\end{pmatrix}\ \ldots\ldots(13)$$

III RESULT AND DISCUSSIONS

Now the frequency of vibration of carbon nanotube for different diameter and corresponding length are theoretically calculated through thin shell model and Weak interaction method in different atomic orders (m, n).

Poisson's ratio, v = 0.1 to 0.54, h= 0.0612nm, ρ = 0.69nm and value of used diameter d = 6.8664× $10^{-10}m$ = 0.68664 nm, frequency f = 12.3445 MHz through shell model while in weak interaction method it is 18.533 MHz. for the order (1, 1). It is now clear that frequency of vibration through weak interaction method is greater to provide expected result so as to design an efficient device. It is also clear from graphical variation that frequency of vibration goes on increasing from shell model to weak interaction method.

TABLE 1 weak interaction method

S. N.	Atomic order (m, n)	Length of tube, L In nm	Tube diameter d_t=o(omicron) √(m²+mn+n²)	Frequency f= $\frac{L}{d_t}$ in mega Hz.
1	(1, 1)	3.21	1.732	18.533
2	(2,2)	0.8044	3.46	2.324
3	(3, 3)	0.3566	5.196	0.686
4	(4,4)	0.20058	6.928	0.2895
5	(5, 5)	0.1283	8.66	0.1482
6	(6, 6)	0.08909	10.392	0.085
7	(7,7)	0.06545	12.124	0.053
8	(8,8)	0.05011	13.856	0.036
9	(9, 9)	0.0395	15.588	0.025
10	(10,10)	0.0311	17.32 0.018	

A graph between nanotube diameter and frequency

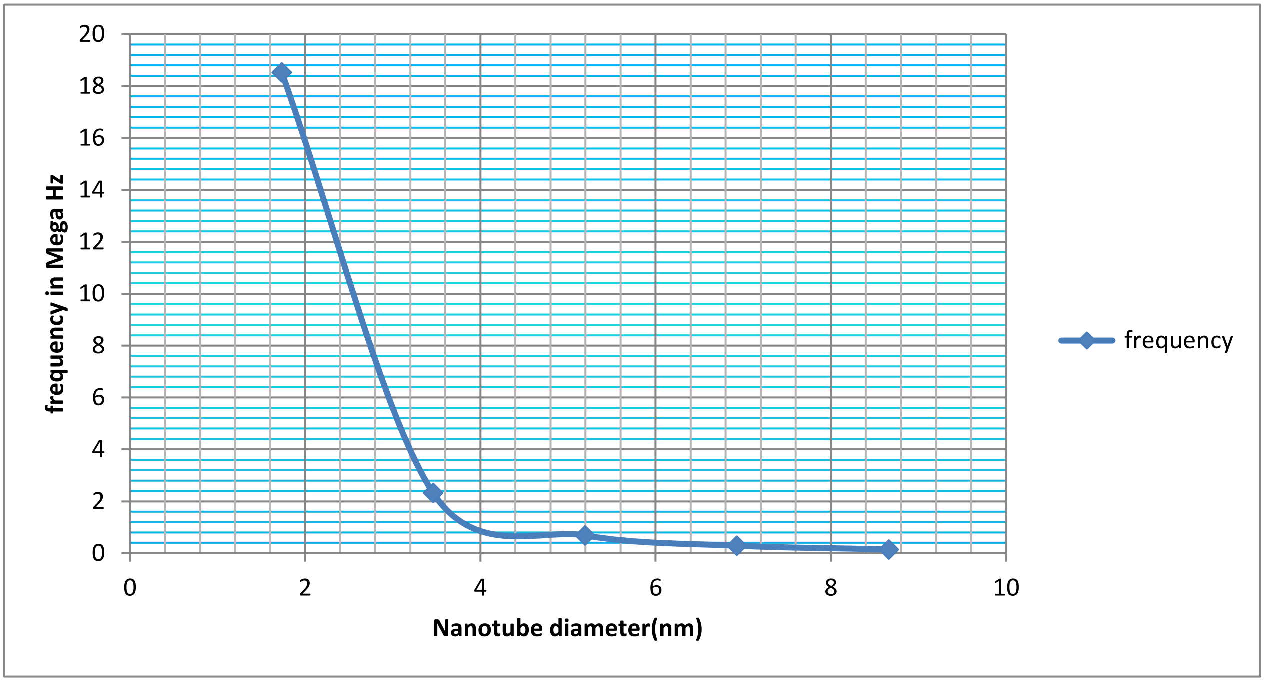

Fig1: variation in frequency versus nanotube diameter (nm)

Table 2: Thin Shell model

S .N	(m, n)	L/d	Frequency
1	(1,1)	4.68	1.17470
2	(4,4)	6.67	0.59090
3	(7, 0)	8.47	1.87
4	(9, 0)	10.26	0.34940
5	(12,12)	13.89	-5.19

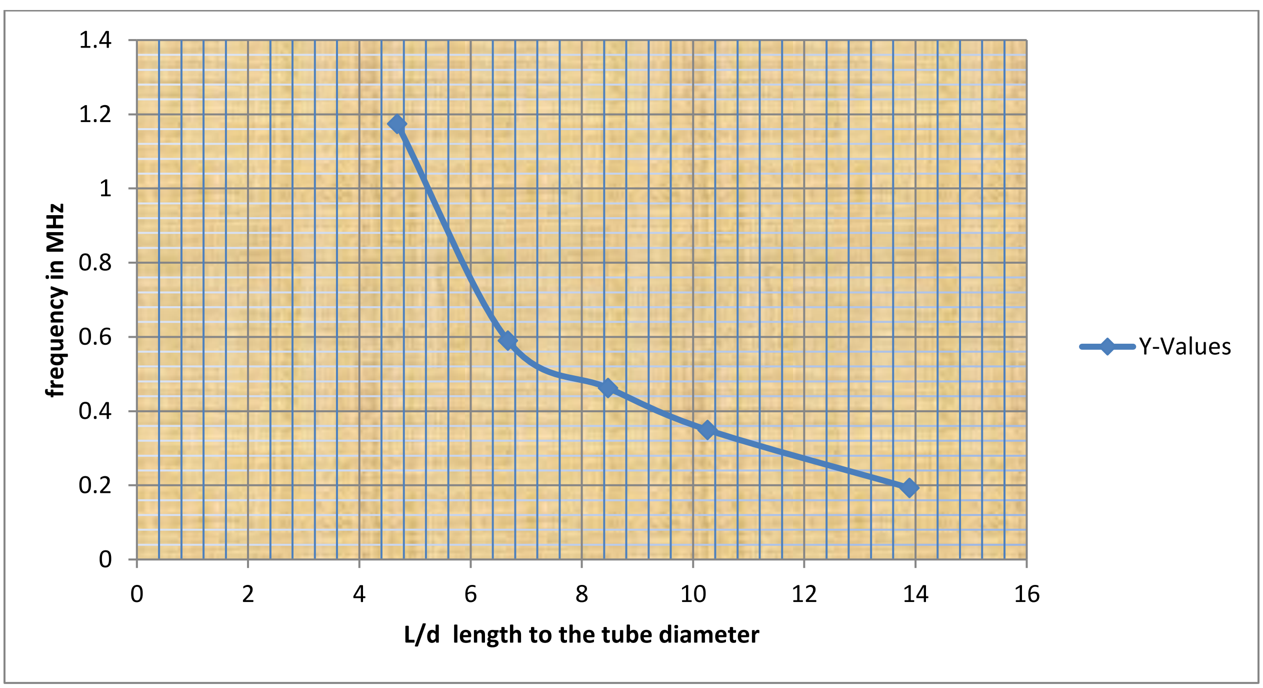

Fig 2: L/d along X- axix and frequency along Y axix.

IV CONCLUSION

A comparative study between weak interaction method and Donnel thin shell model leads to explain frequency of vibration of carbon nanotube can be calculated in accurate way ensuring vibrational properties of CNT . The active device can be designed without much more difficulty and turning to the constructing mode , such as electronic, optical, medicine, charge detectors, sensors, field emission devices, aerospace, defence construction and even fashion[1].

V ACKNOWLEDGEMENT

I thank the Great Nobel Prize winner S.Iijima‟s works on carbon nanotube [4] and Work of Donnel thin shell model. I am also thankful to Prof. Abdus Sattar, H.O.D, Dept. of Physics S.K.M.U. Dumka who inspired me to work continuously to seek innovative thought and achieve new result.

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