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A Numerical Study on the Effect of Length on Natural Frequency of Single Walled Carbon Nanotubes

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Abstract - *Carbon Nanotubes have exceptional mechanical, thermal and electrical properties which makes them highly useful in modern day applications. Depending on the field in which they are used, they might be subjected several vibrations making it very essential to understand their natural frequencies beforehand so that any chance of resonance can be avoided. In this paper, natural frequencies of single walled carbon nanotubes of different chiralities are found out . Variation in frequency with length is also studied in this numerical study performed using ANSYS APDL.*

Key Words*: *Carbon Nanotube, Chirality, Length, Modal Analysis, Frequency, ANSYS APDL

1. INTRODUCTION

Carbon nanotubes (CNTs) are one of the allotropes of carbon which is made of carbon atoms arranged into a continuum of condensed benzene rings (graphene sheets) which is then rolled to form a cylindrical structure[1]. It is the third allotrope of carbon after diamond and graphite. These tube like structures have diameter in nanometre scale and possess extraordinary mechanical, thermal and electrical properties.

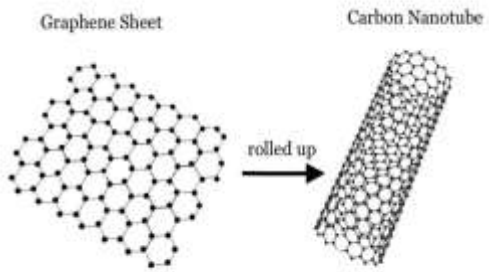

Fig-1. Rolling of graphene sheet into carbon nanotube (Source:Lucy Zuo,2018)

CNTs are one of the strongest and stiffest materials having tensile strength(around 45GPa, 40 times that of steel)and elastic modulus(around 1TPa, 5 times that of steel)[2]
They are classified into two based on their structure: Single-Walled Carbon Nanotube(SWCNT) and Multi-Walled Carbon Nanotube(MWCNT). SWCNT consists of single cylindrical graphene layer which is capped at both ends and has an outer diameter ranging from 1-3nm and inner diameter ranging from 0.6-2.4nm. MWCNTs consist of several concentric layers of graphene sheets and having an outer diameter ranging from 2.5-100nm and inner diameter ranging from 1.5-15nm. MWCNTs comprises of many number of concentric SWCNT layers that are separated by a distance of around 0.34nm[3].

Fig-2.a)Single Walled Carbon Nanotube b)Multiwalled Carbon Nanotube (Source: Toraman et al.,2017)

CNTs have high mechanical, tensile strength, high electrical, thermal conductivity and are ultra-light weight. They are also capable of penetrating many types of cell membranes through passive and endocytosis process. Also CNTs exhibit properties that are desirable for efficient drug delivery system and can be efficiently used for pharmaceutical applications[4].

1.1 Chirality of a CNT

Chirality of a carbon nanotube is defined as the specific angle in which the graphene layers are rolled to form the nanotube structure. It is either represented as an angle or as chiral vectors (n,m). CNTs are thus classified into three based on its chirality namely zig-zag, armchair and chiral.

Zig zag has a chiral angle of 0^0 and is also represented in the form (n,0) whereas armchair has a chiral angle of 30^0 and is of the form (n,n) .i.e ,n=m. Carbon nanotubes having any chiral angle between 0^0 and 30^0 is known as chiral and is of the form (n,m)[5].

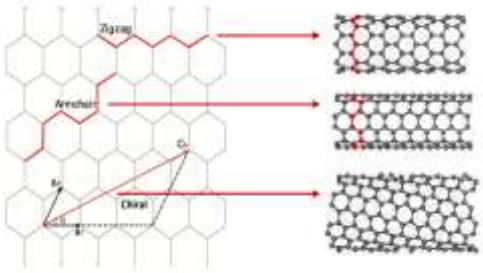

Fig-3. Schematic diagram showing zigzag, armchair and chiral carbon nanotubes (Source: Rahmandoust et al.,2011)

The bond lengths and bond angles are all different for a chiral nanotube whereas there are two unequal parameters for both zigzag and armchair carbon nanotubes [6]

Diameter of a carbon nanotube is given by[7] as,

$D = A/\pi$,

where A is the perimeter vector which is given by

$A = a_o (n^2 + m^2 + nm)^{1/2}$,where a is the chiral vector

Which implies,

$D = a_o (n^2+m^2+nm)^{1/2}/\pi$

1.2 Literature Review

Predicting the mechanical properties had been a complex task for researchers.In a study by Pipes et al., 2002[8], an attempt was made to derive analytical expressions for young's modulus, density and weight volume fraction. These expressions were derived as functions of either chiral vectors or as nanotube radius. Various experimental studies came up with results showing great variation in mechanical properties of the carbon nanotube. This could be because of different assumptions made initially by researchers or could be due to different modeling techniques adopted (Zhang et al., 2005)[9]

Elastic properties of single walled carbon nanotube was studied using Molecular Dynamics simulation(Tahreen et al., 2012)[2]. The study was performed on carbon nanotubes of different length, tube radius and chirality. The results showed that the axial young's modulus reduces as there is an increase in tube radius. Also the study found out that length and chirality had no effects on the same.

Another study (Cao et al., 2007)[10] was focused on the variation of buckling behavior and elastic properties of SWCNT with respect to chirality and boundary conditions. The tube length and diameter was also varied to look into its effects. It was found that both tube chirality and boundary conditions had only considerable influence when the deformation occurred is very large upon both compression and bending. Thus it was concluded that continuum thin shell model is very much suited for modeling nanotube elastic properties.

Molecular dynamics simulation studies the variation in a system with respect to time and is based on both interatomic forces and on Newtonian mechanics .In one another study using MD simulation(Mashreghi et al., 2011)[6], nanotubes having a constant n+m values, nanotube radius reduced as there was an increase in chiral angle.

A new method, namely, Molecular mechanics was employed by Ferreira et al., 2008[11]. In this method, both molecular dynamics and solid mechanics. This new method was checked for all three basic chiralities namely zigzag, armchair and chiral nanotubes. Results obtained were in the range of that in literature. Generally molecular mechanics refers to the study of movement of atoms within a molecule(Rossi et al., 2006)[12].

Carbon nanotubes can be modeled in several ways for the purpose of analysis. Mechanical behavior of isolated single walled carbon nanotube was studied by modeling bonds between two carbon atoms as beam 188 element in ANSYS (Mohammadpour et al.,2012)[13]. The idea of equivalence of energy between structural mechanics and molecular dynamics with the help of modified Morse potential was used to finalize the beam element properties. By this method the young's modulus was found out to be 5.5TPa.

Another study(Hossein et al., 2011)[14]used beam elements for interatomic interactions and non linear spring elements were employed to simulate the Van der Waals bonds. Rossi et al., 2006[12], used non linear and torsional spring elements for finding the mechanical properties of carbon nanotubes. The intention was to incorporate rotational degrees of freedom. The results obtained were in agreement with that of literature.

Another approach for analyzing carbon nanotubes especially when used as a composite is by generating a RVE(Representative Volume Element). Stress distribution of carbon nanotube based aluminum composite for varying CNT bundle was studied using RVE(Chowdhury et al., 2012)[15]. From the study it was revealed that as the distance of the center of CNT from the reference point increases, the stress is found to be decreasing. In another study by Roozpeikar et al., 2018[16], a three dimensional cylindrical RVE was modelled using ABAQUS to study the mechanical properties of composites based on CNT. It was found that even for a very less replacement of carbon nanotube inside the matrix, there is a large improvement in overall stiffness.

A vibrational analysis of single walled carbon nanotubes was conducted (Arghavan et al., 2011)[17] in which actual atomic configuration was modelled. Analysis was performed on both zigzag and armchair for clamped-clamped and clamped-free boundary conditions and their natural frequencies and their respective mode shapes were obtained. It was found that the nanotube behaved

just as that of a cylindrical shell and is almost impossible to distinguish them visually.

In a study by Mir et al.(2009)[18], six carbon nanotubes were analysed and their natural frequencies were extracted. The analysis were performed for three different lengths, 15nm, 20nm and 25nm. It was found that the frequency decreased with respect to increase in length.

The above mentioned study considered only three lengths of carbon nanotubes. It would have provided a clear image if more number of lengths were considered. In this study, carbon nanotubes of a larger number of lengths (ranging from 5nm to 100nm) were analyzed in order to study the trend.

2. MODELING OF CARBON NANOTUBE

In this study, carbon nanotubes were modeled and simulated using ANSYS APDL 16.0. Carbon atoms are considered to act as a lumped mass having magnitude equivalent to that of a real carbon atom (1.996 x 10^{-26} kg),which is mainly the sum of six protons and six neutrons consisting in a carbon atom) and covalent bonds between these atoms are considered to be connected by beam elements. BEAM188 element (a 3-D beam element having six degrees of freedom i.e, three translations and three rotations degrees of freedoms at two end nodes)is used as it is capable for these requirements. Mass of carbon atom is depicted using MASS21 element(a point element having up to six degrees of freedom).

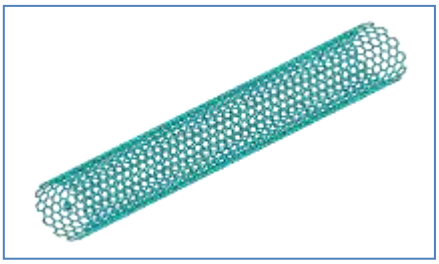

Fig-4. Model of a (12,12) carbon nanotube in ANSYS APDL

The beam element properties are calculated using force field constants . The molecular mechanics constants are given below from experimental data as mentioned in[7]:

k_r = 6.52e-7 N nm^{-1}

k_θ = 8.76e-10 N nm rad^{-2}

k_Φ = 2.78e-10 N nm rad^{-2}

where k_r is the bond stretching stiffness, k_θ is the angle bending stiffness and k_Φ is the torsional stiffness and thickness, t=0.34nm(which is equivalent to the interlayer spacing of graphite)[3] .

Using these constants, the diameter(d), Young's modulus(E) and shear modulus(G) are computed using following equations as suggested by Sakhaee-Pour et.al (2009)[19].

$d=4(k_\theta/k_r)^{1/2}$

$E=(k_r^2 L/4\Pi k_\theta)$

$G=(k_r^2 k_\Phi L/8k_\theta^2)$

The calculated values of d, E and G respectively are 0.1466 nm, 5.48 x 10^{12} N/m^2 and 0.871 x 10^{12} N/m^2. A density of 2.3 g/cm3 is also provided to the beams as suggested by Mir et al.,(2007)[18].

2.1 Scaling of the Model

Since carbon nanotubes are having dimensions in the range of 10^{-9}, analysis cannot be directly performed in ANSYS APDL. Thus scaling of the model becomes necessary. Geometric similarity property as proposed by Mir et al.[18] is adopted here. For a model scaled up by a factor of $\beta=l/L$, where l is the actual length and L is the length of the model structure, then their respective frequencies are related by $\omega_1 = \omega_2/\beta$, where ω_1 and ω_2 are respectively the model frequency and actual frequency.

3. ANALYSIS AND RESULTS

Modal analysis was performed on several single walled carbon nanotubes of different chiralities. Two different boundary conditions were considered, namely cantilever (Clamped-Free) and bridge (Clamped-Clamped) condition. Initially validation was done so as to confirm that the modeling techniques adopted were correct. Values obtained in this section was in agreement with previous studies with only minor errors.

Frequency in GHz	A. Sakhaee-Pour et.al [20]	M. Mir, A. Hosseini, G.H. Majzoobi [18]	*Present Work*
	L=12.305nm, D=0.814nm E=5490 GPa, G=871 GPa,thickness =0.147nm,Mass of carbon atom=1.996x10-26kg		
mode 1	23	28	22.40
mode 2	23	28	22.40
mode 3	138	171	133.59
mode 4	138	171	133.59
mode 5	300	433	228.81

Table -1: Natural frequencies of cantilever (6,6) carbon nanotube

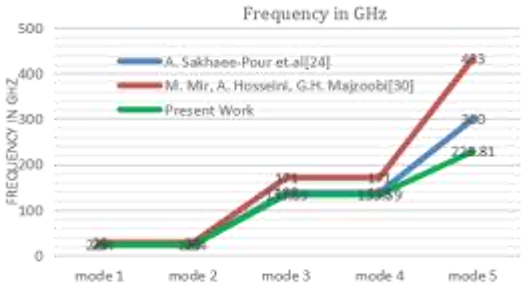

Chart-1: Comparative graph of validation data

In order to study the effect of length on natural frequencies, several carbon nanotube models were analyzed and following results were obtained.

Frequency in GHz	Length of carbon nanotube					
	5nm	10nm	15nm	30nm	50nm	75nm
mode 1	76.71	18.72	8.72	2.18	2.16	2.16
mode 2	76.71	18.72	8.72	2.18	2.16	2.16
mode 3	444.46	114.97	54.15	13.65	13.49	13.49
mode 4	444.46	114.97	54.15	13.65	13.49	13.49
mode 5	585.95	289.38	149.44	38.07	37.63	37.63
mode 6	1019.1	312.47	149.44	38.07	37.63	37.63
mode 7	1129	312.47	197.67	74.2	73.36	73.36
mode 8	1129	500.57	287.05	74.2	73.36	73.36
mode 9	1758	588.66	287.05	99.23	98.422	98.422
mode 10	1982.1	588.66	341.32	121.83	120.46	120.46

Table -2: Natural frequencies of cantilever (6,0) carbon nanotube of different length

Frequency in GHz	Length of carbon nanotube					
	5nm	10nm	15nm	30nm	50nm	75nm
mode 1	517.87	126.44	59.13	14.22	14.11	14.11
mode 2	517.87	126.44	59.13	14.22	14.11	14.11
mode 3	1256	334.8	159.82	39	38.66	38.66
mode 4	1256	334.8	159.82	39	38.66	38.66
mode 5	1312	610.98	305.8	75.98	75.4	75.4
mode 6	2185.7	626.38	305.8	75.98	75.4	75.4
mode 7	2185.7	626.38	411.43	124.64	123.12	123.12
mode 8	2234	983.51	491.3	124.64	123.12	123.12
mode 9	2624	983.51	491.3	184.51	183.11	183.11
mode 10	3232.8	1047.1	709.61	184.51	183.11	183.11

Table -3: Natural frequencies of bridge(6,0) carbon nanotube of different length

Frequency in GHz	Length of carbon nanotube						
	5nm	10nm	12.3nm	15nm	20nm	30nm	50nm
mode 1	139.01	33.37	22.41	22.409	22.432	22.432	22.432
mode 2	139.01	33.37	22.41	22.409	22.432	22.432	22.432
mode 3	583.39	194.57	133.59	133.59	133.73	133.73	133.73
mode 4	686.92	194.57	133.59	133.59	133.73	133.73	133.73
mode 5	686.92	279.83	228.81	228.8	229.1	229.1	229.1
mode 6	1066.1	496.9	349.58	349.58	349.96	349.96	349.96
mode 7	1563.5	496.9	349.58	349.58	349.96	349.96	349.96
mode 8	1563.5	511.55	418.22	418.22	418.69	418.69	418.69
mode 9	1752.9	839.8	631.16	631.16	631.86	631.86	631.86
mode 10	2511.9	876.3	631.16	631.16	631.86	631.86	631.86

Table-4 : Natural frequencies of cantilever (6,6) carbon nanotube of different length

Frequency in GHz	Length of carbon nanotube					
	5nm	12.3nm	15nm	20nm	30nm	50nm
mode 1	687.12	139.9	139.79	137.29	137.29	137.29
mode 2	687.12	139.9	139.79	137.29	137.29	137.29
mode 3	1217.9	354.0	353.69	347.83	347.83	347.83
mode 4	1488.1	354.0	353.69	347.83	347.83	347.83
mode 5	1488.1	470.5	470.04	465.8	465.8	465.8
mode 6	2210.8	633.9	633.3	623.53	623.53	623.53
mode 7	2439.3	633.9	633.3	623.53	623.53	623.53
mode 8	2439.3	860.2	859.33	851.42	851.42	851.42
mode 9	2441.7	941.4	940.46	931.96	931.96	931.96
mode 10	2591.4	956.5	955.54	941.67	941.67	941.67

Table-5 : Natural frequencies of bridge (6,6) carbon nanotube of different length

Frequency in GHz	Length of carbon nanotube						
	5nm	10nm	15nm	20nm	30nm	40nm	50nm
mode 1	100.87	27.08	11.59	6.39	2.87	2.87	2.87
mode 2	100.87	27.08	11.59	6.39	2.87	2.87	2.87
mode 3	550.54	162.75	71.32	39.68	17.87	17.89	17.89
mode 4	550.54	162.75	71.32	39.68	17.87	17.89	17.89
mode 5	574.86	296.33	193.86	109.4	49.7	49.76	49.76
mode 6	1024.3	430.23	194.37	109.4	49.7	49.76	49.76
mode 7	1327.3	430.23	194.37	144.05	96.39	96.517	96.517
mode 8	1327.3	525.25	342.89	209.85	96.42	96.529	96.529
mode 9	1724.9	785.1	367.35	209.85	96.42	96.529	96.529
mode 10	2230.8	785.1	367.35	254.51	157.41	157.58	157.58

Table-6 : Natural frequencies of cantilever (8,0) carbon nanotube of different length

Frequency in GHz	Length of carbon nanotube						
	5nm	10nm	15nm	20nm	30nm	40nm	50nm
mode 1	623.02	177.95	76.43	41.58	18.563	18.714	18.714
mode 2	623.02	177.95	76.43	41.58	18.863	18.714	18.714
mode 3	1287.6	454.66	203.24	112.34	50.7	51.104	51.104
mode 4	1425.4	454.66	203.24	112.34	50.7	51.104	51.104
mode 5	1425.4	627.27	381.83	214.81	98.23	99	99
mode 6	2246.5	821.82	381.83	214.81	98.23	99	99
mode 7	2396.5	821.82	402.24	293.5	160.08	161.31	161.31
mode 8	2396.5	1101.9	601.85	344.83	160.08	161.31	161.31
mode 9	2576.2	1250.6	601.85	344.83	195.19	196.57	196.57
mode 10	3453.9	1250.6	707.57	498.6	235.22	237	237

Table-7 : Natural frequencies of bridge (8,0) carbon nanotube of different length

	Length of carbon nanotube								
	5nm	10nm	20nm	30nm	40nm	50nm	60nm	80nm	100nm
mode 1	240.7	63.83	16.28	7.36	4.07	2.68	1.85	1.04	0.645
mode 2	240.7	63.83	16.28	7.36	4.07	2.68	1.85	1.04	0.65
mode 3	586.7	281.43	95.02	44.61	25.04	16.59	11.51	6.48	4.06
mode 4	691.9	318.53	95.02	44.61	25.04	16.59	11.51	6.48	4.06
mode 5	691.9	318.53	139.6	93.6	68.16	45.59	31.79	18.03	11.3
mode 6	896.4	513.85	242.8	119.1	68.16	45.59	31.79	18.03	11.3
mode 7	896.4	682.17	242.8	119.1	69.54	56.41	46.87	34.96	22
mode 8	897.4	682.17	254.7	170.7	126.7	87.05	61.15	34.96	22
mode 9	897.4	711.7	418.9	219.6	128.6	87.05	61.15	35.13	27.75
mode 10	1067	711.7	428.3	219.6	128.6	102.8	85.39	57.02	36.06

Table-8 : Natural frequencies of cantilever (12,12) carbon nanotube of different length

	Length of carbon nanotube								
	5nm	10nm	20nm	30nm	40nm	50nm	60nm	80nm	100nm
mode 1	833.5	309.6	95.73	45.34	25.51	16.92	11.73	4.13	95.73
mode 2	833.5	309.6	95.73	45.34	25.51	16.92	11.73	4.13	95.73
mode 3	873.6	574.33	235.8	117.7	67.87	45.54	31.8	11.33	235.83
mode 4	873.6	672.18	235.8	117.7	67.87	45.54	31.8	11.33	235.83
mode 5	1224	672.18	282.0	188.4	127.5	86.66	61.02	22.03	282.01
mode 6	1366	706.63	413.2	215.6	127.5	86.66	61.02	22.03	413.2
mode 7	1366	706.63	413.2	215.6	139.7	113.3	94.05	36.07	413.2
mode 8	1681	794.94	514.9	331.6	200.9	138.4	98.36	36.07	514.91
mode 9	1681	794.94	564.1	331.6	200.9	138.4	98.36	53.27	564.11
mode 10	1952	970.65	612.7	343.9	254.9	198.9	142.8	53.27	612.72

The above data are represented using bar chart below for convenient comparisons.

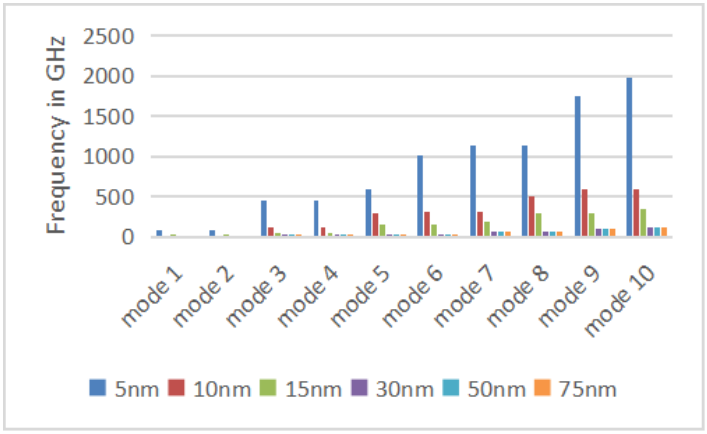

Chart -2: Natural frequencies of cantilever (6,0) carbon nanotube of different length

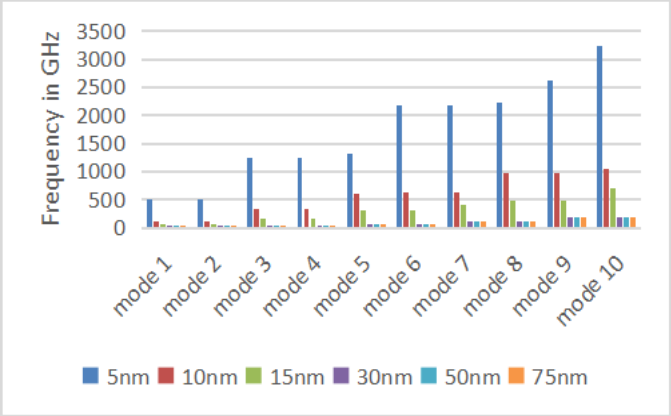

Chart -3: Natural frequencies of bridge(6,0) carbon nanotube of different length

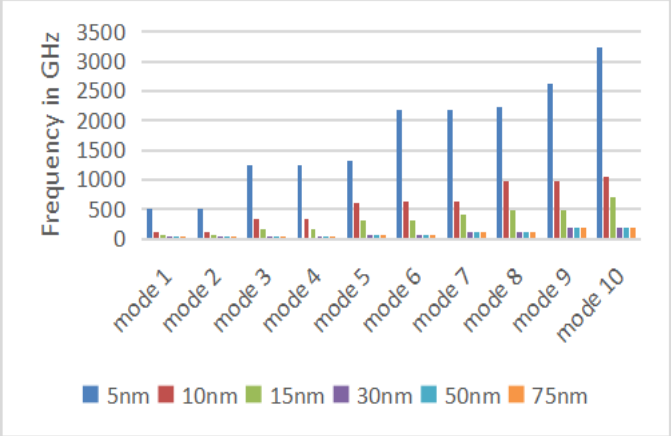

Chart-4 : Natural frequencies of cantilever (6,6) carbon nanotube of different length

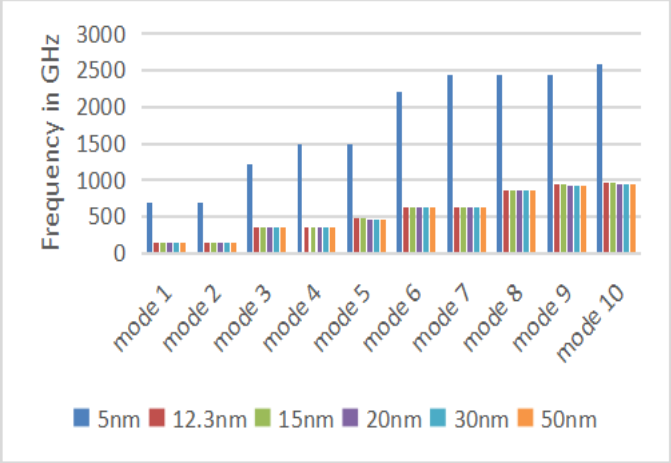

Chart-5 : Natural frequencies of bridge (6,6) carbon nanotube of different length

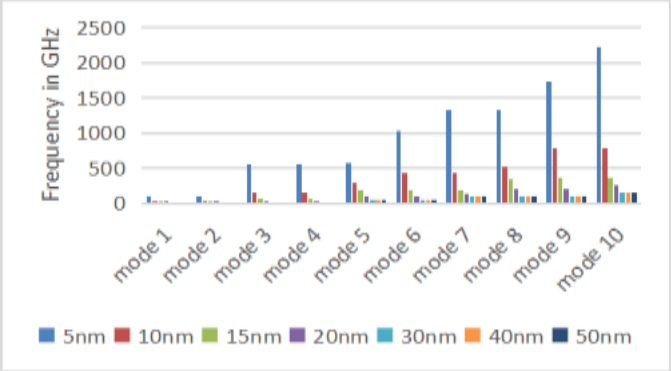

Chart-6 : Natural frequencies of cantilever (8,0) carbon nanotube of different length

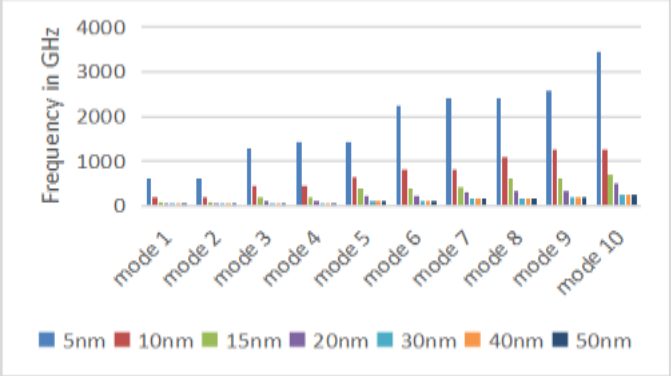

Chart-7 : Natural frequencies of bridge (8,0) carbon nanotube of different length

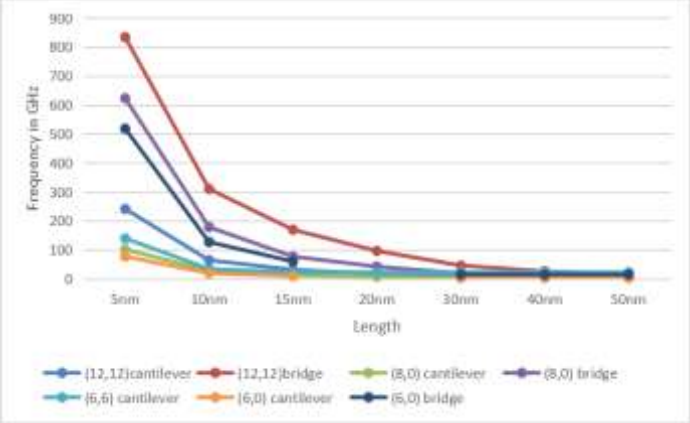

Chart-8 : Mode 1 frequencies of different carbon nanotube models

4. CONCLUSIONS

- From charts 1 to 7, it can be concluded that the natural frequencies decreases as length increases and converges to a specific frequency at some length(depicted by bars of similar heights at the end).
- Carbon nanotubes of smaller diameter converges at an earlier point compared larger diameter ones as it is evident from chart-8.

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