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Characterization of Single Walled Nanotube Using Finite Element Method

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Abstract — **The mechanical properties of carbon nanotube are investigated and shed a new light on the nature of stress production and relaxation of carbon nanostructures. The behavior of the carbon nanotubes are analyzed based on the modulus of elasticity , the strain of the tube with the applied stress in steps and its deformation(elongation) with the given stress have been analyzed using 'Finite' element method . And also the responses with the finite element method are analyzed using different wall thickness. The calculated results for both armchair and Zig- Zag Single walled carbon nanotubes exhibits very high mechanical strength and it observed that at very high load inputs at both ends, Kinks and buckling are formed and later it tends to collapse.**

I. INTRODUCTION

In recent developments the technology is focusing on the Nanotubes, and Nano materials. Considering the elasticity and ductileness, Nanotubes are having its unique significance in medical, water purification and in defense applications. Space frame like structure is simulated. The carbon Nano tubes acts as joints to the connecting atoms. The covalent bond between the carbon atoms considered as connecting elements. The bonds between the carbon atoms modeled as elastic beam elements. For analyzing the nano tubes, FEM and molecular dynamics (MD) tools are widely used. Carbon nanotubes are classified as single walled carbon nanotubes (SWCNTS) and multi walled carbon nanotubes (MWCNTs).

A thin graphite sheet rolled into a cylindrical shape, a hallow structure is formed by the carbon atoms with covalently bonded. The end caps (hemispherical caps) used to seal both ends of the CNTs. Long continuous CNTs can be formed by neglecting the end caps and considering the length to diameter aspect ratio. The angle subtended by rolling the graphite sheet may form armchair, Zig-Zag, Chiral type of nanotubes. A Vector (n,m) is used to describe the structure of the Nanotubes. For all Zig-Zag tubes m=0, for all armchair tubes n=m and for all chiral tubes n,m are different.

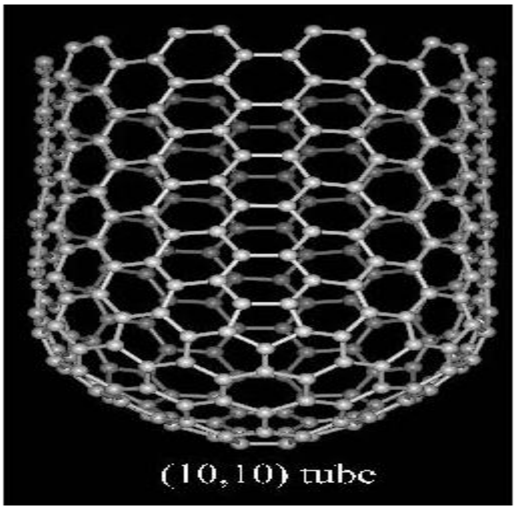

Figure1. Single walled carbon nanotube

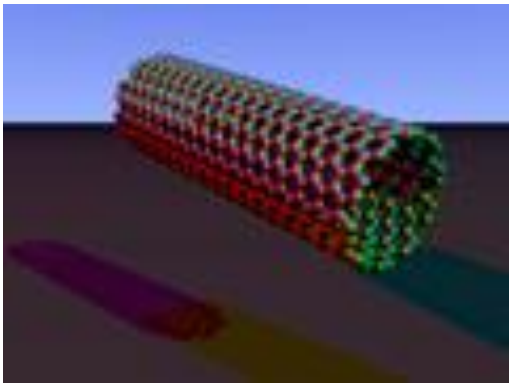

Figure 2. Armchair nanotube with indices (n,n)

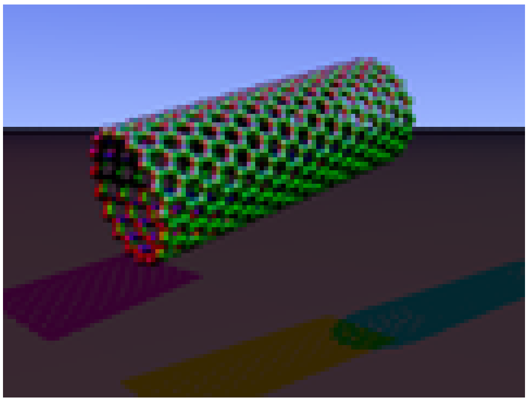

Figure.3 Zig-Zag nanotube with indices (n,0)

The distribution of stress on CNTs and its structural bend, twist is analyzed using the proposed FEM. The modulus of elasticity for various lengths of the tubes for both armchair and Zig-Zag carbon Nanotubes are observed.

II. Related work

This study focused to develop a single walled carbon nanotube by bending the graphite sheet at its vertical edge [1].

The study is focused on Dynamics analysis of single boron nitride nanotubes (SWBNNT) as a resonant nano mechanical sensor by using the finite element method. the intermediate landing position of the added mass is analyzed[2].

The study is focused on the influence of young's modulus on single walled carbon nanotubes of armchair and Zig-Zag for different wall thickness and with different loading conditions [3].

The simulation was conducted by fixing the one end and on the other end an axial tensile strain is applied to observe the response of the nanotube . The young's modulus is estimated accordingly. The Zirconium tubes are significantly affected with diameter, thickness and length changes [4].

This paper presents theory of micro nano mechanics, numerical analysis of mechanical properties characterization. In Finite element modeling three different approaches discussed [5]

Finite element method is adopted to analyze the flexural vibrations of SWCNTs. Shear deformation and an axial deformation of the nanotube is considered for formulation. This paper described the initial stress influence on the natural frequency of the nanotube [6].

III. Methodology

Declaration and Estimation of the parameters

Step1: Declare the length of the tube before the tube is deformed its shape.

Step2: The thickness of the nano tube is taken using previous experiments

Where, t = 0.1296*10-9 meters

Step3: The radius is determined with fixed length and thickness for both armchair, and Zig-Zag nano tubes

For armchair, ranging from 0.673 to 6.732 for (1,1) to (10,10) nanotube

For zig-zag, ranging from 0.389 to 4.276 for (1,0) to (11,0) nanotube

The parameters are calculated by assuming the applied force to the tube in steps of 1 N/M2 and up to 5.5 N/M 2

Stress=force/area, Where, area=pi*d*t, d=diameter of the tube

Step4: Young's modulus is to be considered from the estimated value in MD simulations (which is determined) taken as reference value to find the stress and strain in finite element modeling. Strain of the nanotube is calculated using the formula

Strain=stress * young's modulus.

By using the calculated strain Values, calculate the final length of the tube

Step5: Final length, L2=strain*(1+L1)
Where L1 is the initial length,
Determined the value of bond length (W) of nanotube as 3.40A. Moment of inertia can be calculated by using

I= W*r3

Where, r= radius of the tube,
By using the calculated value of moment of inertia, have been calculated the stiffness constant of the tube.

Stiffness constant, K= y*I/L
Where y= young's modulus
L= L2-L1= change in length.

IV. Results and analysis

FEM Simulations for ARMCHAIR Nanotube
Thickness=0.1296nm, Initial length,

L1=30, Bond angle W= 3.40A.

Radius (r)	Area	Force (f)	Stress (s)	Final length (L2)	Change in length ΔL	Strain (e)	young's modulus Y	Moment of inertia I	Bending stiffness K
0.6730	0.5477	1	1.8257	39	9.0000	0.3000	6.0855	0.001	0.7008
1.3460	1.0955	1.5	1.3692	39.81	9.81	0.3270	4.1873	0.0083	3.5390
2.0190	1.6432	2.0	1.2171	40.62	10.62	0.3540	3.4382	0.028	9.0592
2.6920	2.1910	2.5	1.1410	41.43	11.43	0.3810	2.9949	0.0663	17.379
3.3650	2.7387	3.0	1.0954	42.24	12.24	0.4080	2.6848	0.1295	28.416
4.0380	3.2865	3.5	1.0650	43.05	13.050	0.4350	2.4482	0.2239	41.996
4.7110	3.8342	4.0	1.0432	43.86	13.860	0.4620	2.2581	0.3555	57.915
5.3840	4.3820	4.5	1.0269	44.67	14.67	0.4890	2.1001	0.5306	75.962
6.0570	4.9297	5.0	1.0143	45.48	15.48	0.5160	1.9656	0.7555	95.935

Table1. Mechanical parameters estimated for armchair carbon nanotubes

FEM Simulations for ZIG-ZAG Nanotube

Initial length, L1=30, bond angle W=3.40A

Radius (r)	Area	Force (f)	Stress (s)	Final length(L2)	Change in length ΔL	Strain (e)	young's modulus Y	Moment of inertia I	Bending stiffness K
0.3890	0.3166	1.0000	3.1585	45.9	15.9000	0.5300	5.9595	0.2001	0.0750
0.7780	0.6332	1.5000	2.3689	47.3	17.3000	0.5767	4.1079	1.6011	0.3802
1.1670	0.9498	2.0000	2.1057	48.7	18.7000	0.6233	3.3781	5.4037	0.9762
1.5560	1.2664	2.5000	1.9741	50.100	20.1000	0.6700	2.9464	12.8088	1.8776
1.9450	1.5830	3.0000	1.8951	51.5	21.5000	0.7167	2.6444	25.0171	3.0769
2.3340	1.8996	3.5000	1.8425	52.90	22.9000	0.7633	2.4137	43.2296	4.5565
2.7230	2.2162	4.0000	1.8049	54.300	24.3000	0.8100	2.2282	68.647	6.2947
3.1120	2.5328	4.5000	1.7767	55.70	25.7000	0.8567	2.0739	102.470	8.2692
3.5010	2.8494	5.0000	1.7547	57.10	27.1000	0.9033	1.9425	145.94	10.4581

Table 2. Mechanical parameters for zigzag carbon nano tubes

ARMCHAIR: Initial length, L1=30 ,Thickness=0.34nm,

Radius (r)	Area	Force (f)	Stress (s)	Final length (L2)	Change in length ΔL	Strain (e) ΔL/L1	young's modulus Y	Moment of inertia I	Bending stiffness K
0.6730	1.4370	1.0000	0.6959	39.000	9.0000	0.3000	2.3197	0.001	0.0267
1.3460	2.8740	1.5000	0.5219	39.810	9.8100	0.3270	1.5961	0.0083	0.1349
2.0190	4.3110	2.0000	0.4639	40.620	10.6200	0.3540	1.3105	0.028	0.3453
2.6920	5.7480	2.5000	0.4349	41.430	11.4300	0.3810	1.1416	0.0663	0.6625
3.3650	7.1849	3.0000	0.4175	42.240	12.2400	0.4080	1.0234	0.1295	1.0832
4.0380	8.6219	3.5000	0.4059	43.050	13.0500	0.4350	0.9332	0.2239	1.6008
4.7110	10.0589	4.0000	0.3977	43.860	13.8600	0.4620	0.8607	0.3555	2.2076
5.3840	11.4959	4.5000	0.3914	44.670	14.6700	0.4890	0.8005	0.5306	2.8955
6.0570	12.9329	5.0000	0.3866	45.480	15.4800	0.5160	0.7492	0.7555	3.6568
6.7300	14.3699	5.5000	0.3827	46.290	16.2900	0.5430	0.7049	1.0364	4.4845

Table 3. Mechanical parameters estimated with thickness 0.34nm for armchair carbon nano tubes

ZIG-ZAG: Initial length=30, Thickness =0.34nm

Radius(r)	Area	Force (f)	Stress (s)	Final length (L2)	Change in length ΔL	Strain (e)	young's modulus Y	Moment of inertia I	Bending stiffness K
0.3890	0.8306	1.0000	1.2040	45.9	15.9000	0.5300	2.2716	0.2001	0.0286
0.7780	1.6612	1.5000	0.9030	47.3	17.3000	0.5767	1.5658	1.6011	0.1449
1.1670	2.4918	2.0000	0.8026	48.7	18.7000	0.6233	1.2877	5.4037	0.3721
1.5560	3.3224	2.5000	0.7525	50.100	20.1000	0.6700	1.1231	12.8088	0.7157
1.9450	4.1530	3.0000	0.7224	51.5	21.5000	0.7167	1.0080	25.0171	1.1729
2.3340	4.9836	3.5000	0.7023	52.90	22.9000	0.7633	0.9201	43.2296	1.7368
2.7230	5.8141	4.0000	0.6880	54.300	24.3000	0.8100	0.8494	68.647	2.3994
3.1120	6.6447	4.5000	0.6772	55.70	25.7000	0.8567	0.7905	102.4702	3.1520
3.5010	7.4753	5.0000	0.6689	57.10	27.1000	0.9033	0.7404	145.94	3.9864
3.8900	8.3059	5.5000	0.6622	58.50	28.5000	0.9500	0.6970	200.1372	4.8948

Table 4. Mechanical parameters estimated with thickness 0.34nm zigzag carbon nanotubes.

FEM Simulations, For Thickness=0.1296nm

For ARMCHAIR			For ZIG-ZAG			
Change in length ΔL	Strain (e)	young's modulus Y	Change in length ΔL	Strain (e)	young's modulus Y	Bending stiffness K
9.0000	0.3000	6.0855	15.9000	0.5300	5.9595	0.0750
9.81	0.3270	4.1873	17.3000	0.5767	4.1079	0.3802
10.62	0.3540	3.4382	18.7000	0.6233	3.3781	0.9762
11.43	0.3810	2.9949	20.1000	0.6700	2.9464	1.8776
12.24	0.4080	2.6848	21.5000	0.7167	2.6444	3.0769
13.050	0.4350	2.4482	22.9000	0.7633	2.4137	4.5565
13.860	0.4620	2.2581	24.3000	0.8100	2.2282	6.2947
14.67	0.4890	2.1001	25.7000	0.8567	2.0739	8.2692
15.48	0.5160	1.9656	27.1000	0.9033	1.9425	10.4581

Table5. change in length and strain for armchair and Zig-Zag carbon nano tubes.

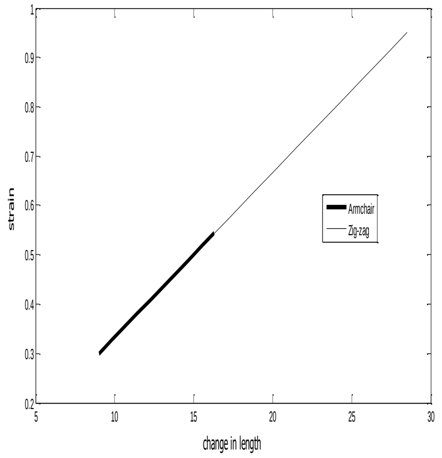

Figure 4 Change in length Vs. strain for both Armchair and Zigzag

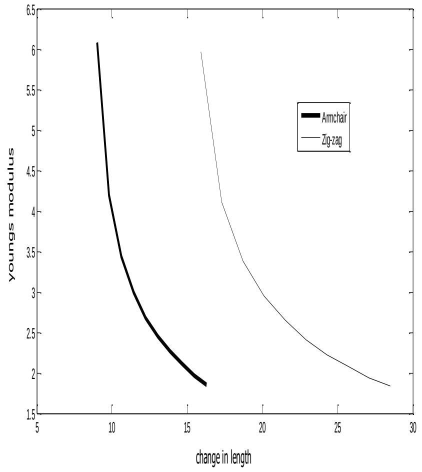

Figure 5 .change in length vs. youngs modulus for both armchair and zigzag carbon nanotubes.

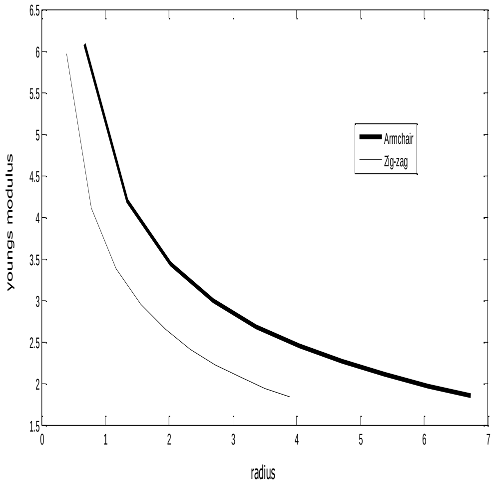

Figure 6. radius vs young's modulus for both armchair and zigzag carbon nanotubes.

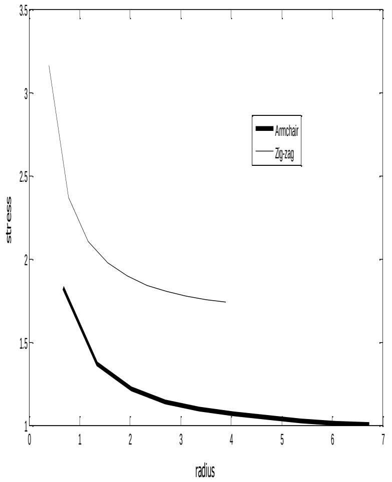

Figure 7. radius vs stress for both armchair and zigzag carbon nanotubes.

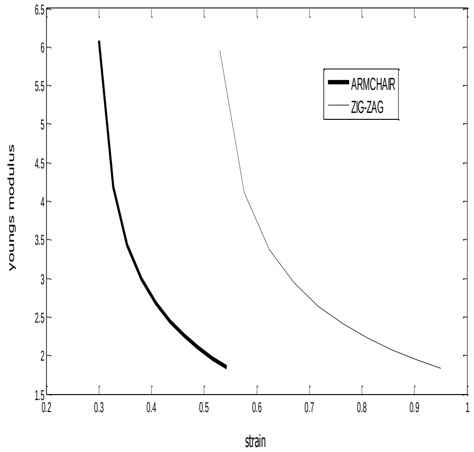

Figure 8. strain vs young's modulus for both armchair and zigzag carbon nanotubes.

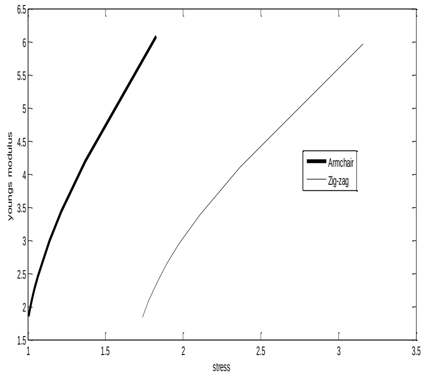

Figure 9. stress vs young's modulus for both armchair and zigzag carbon nanotubes.

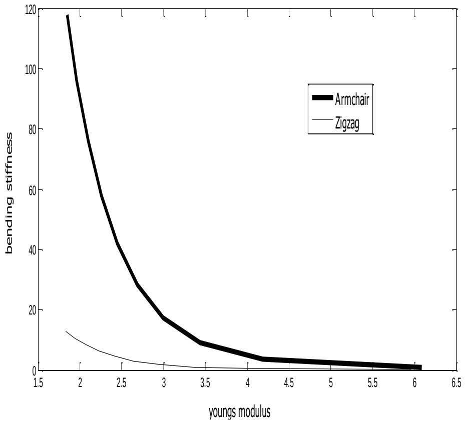

Figure 10. young's modulus vs bending stiffness for both armchair and zigzag carbon nanotubes

The results are depicted for the armchair and zig-zag nanotubes for different wall thickness using Finite Element Model (FEM) and have been compared.

It is observed that a linear stress developed on both armchair and Zig-Zag 'SWCNTs' with small radius of the tube .By increasing the radius of the tube the stress developed is decreasing in parabolic order. And also Kinks are observed when the response of the tube turns from linear to parabolic. More stress developed for Zig-zag 'SWCNTs' rather than Armchair. With increasing the radius, the stress developed in the armchair is closes to zero value. Buckling occurred with the higher strain values.

It is also observed that by neglecting the end caps and increasing the tube length, the strain developed with the applied load is linearly proportional for both armchair and Zig-Zag SWCNTs. The tube tend to bend due to increasing the young's modulus with increasing the length of the tube for both armchair and Zig-zag SWCNTs.

It also observed that the bending stiffness of the Zig-Zag SWCNTs is very small with applied strain. In case of Armchair, the bending stiffness is considerably high for minimum strain applied to the tube. With increasing the strain the bending stiffness is decreased and this response is parabolic for armchair SWCNTs. The stiffness of the zigzag nanotube is little bit higher than the armchair nanotube. As the diameter of the tube increases, the modulus elasticity of the tube decreases. The tube surface area is found to be increased near linearly with increasing axial strain, since the tube diameter increases slightly with tensile Strain.

The values of the stress for different wall thickness have been investigated. Even though, by considering small thickness of the tube, it is to be observed that the tube can withstand to the more stress applied.

As the length of the tube increases by applying strain, the young's modulus of the tube decreases and the bending stiffness increases. As the wall thickness increases its modulus of elasticity decreases. Thus the tube with low wall thickness has higher strength.

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