

Single Walled and Multi Walled Carbon Nanotube Structure, Synthesis and Applications

E.N. Ganesh

Abstract - Carbon Nanotubes have exceptional mechanical and electrical properties. Various methods have been thoroughly investigated for the growth of CNTs. The best and the most commonly used method is Chemical Vapour Deposition (CVD). The various techniques include Reaction Chamber heating, Plasma Enhanced CVD, Hot filament CVD, Microwave CVD. The structural uniformity of carbon nanotubes produced by plasma enhanced Chemical Vapour Deposition gives uniform height and diameter. This paper discusses about all the methods listed above and detail comparisons are listed. We have simulated the single layer and multi layer Carbon nano tube using nano explorer tool and enumerated its properties for various applications like power storage and medical applications. The simulated properties of CNT would be used for energy storage purpose as well for transmission of electrical energy. Though it is known that CNT's have high aspect ratio, Young's modulus over one terra pascal, Tensile strength of 200 Gigapascal, these properties never remain the same for all the CNT'S. It depends upon the method of preparation, catalyst used etc. So the properties of CNT are studied for specific conditions. Here it is proposed CNT can be modeled for particularly electrical storage purpose.

Index Terms – Carbon nanotube, chemical vapour deaposition, Plasma enhanced CVD, Multiwall nano tubes.

1 INTRODUCTION

In the recent years miniaturized components plays important role in all type of applications. One such structure is carbon nanotube; Carbon nanotubes (CNTs) are hollow cylinders of carbon atoms. Their appearance is that of rolled tubes of graphite, such that their walls are hexagonal carbon rings, and they are often formed in large bundles. The ends of CNTs are domed structures of six-membered rings, capped by a five-membered ring. There are two types of nanotubes: single-walled nanotubes (SWNTs) and multiwalled nanotubes (MWNTs), which differ in the arrangement of their graphene cylinders. SWNTs have only one single layer of graphene cylinders; while MWNTs have many layers (approximately 50) [1] [2]. There are three types of nanotubes, armchair, zigzag, and chiral. Carbon nanotubes can be either a metal or a semi-conductor. They differ symmetrically and can vary in function due to the way they “roll up.” The diameter of a carbon nanotube can be 50,000 times thinner than a human hair yet a nanotube is stronger than steel per unit weight. This paper discusses

1). Comparison of different methods about synthesis of carbon nano tube

2) study of structure of SWNT, DWNT and MWNT carbon nano tube and calculated structure related parameters of three types of CNT's

3). Simulation of carbon nano tubes with different distortions

4) study about the properties of carbon nano tube for Energy storage and Medical applications.

II CARBON NANOTUBE SYTHESIS – COMPARISON

Generally, three techniques are being used for producing CNTs: 1) the carbon arc-discharge technique [3], [4][5]; 2) the laser-ablation technique [6][7]; and 3) the chemical vapor deposition (CVD) technique [8]–[9]. Among the CNTs, MWNTs were first discovered by Iijima in 1991 by the arc-discharge method [3]. After two years, Iijima and Ichihashi [10] and Bethune *et al.* [11] produced SWNTs. The SWNTs were produced using metal catalyst in the arc-discharge method. Thess *et al.* [6] synthesized bundles of aligned SWNTs by the laser-ablation technique. For the first time, catalytic growth of MWNTs by CVD was proposed by Yacaman *et al.* [8]. The arc-discharge technique produces high quality MWNTs and SWNTs. MWNTs do not need a catalyst for growth, while SWNTs can only be grown in the presence of a catalyst in this method. First time, Ebbesen and Ajayan [12] synthesized high-quality MWNTs having diameters in the range of 2–20 nm and lengths of several micrometers at the gram level. SWNTs produced by laser-ablation were ropes (or bundles) of 5–20 nm diameter and tens to hundreds of micrometers. SWNTs produced by laser-ablation were ropes (or bundles) of 5–20 nm diameter and tens to hundreds of micrometers of length. When synthesizing SWNTs, the by-products in the case of the arc-discharge and laser-ablation techniques are fullerenes, graphitic polyhedrons with enclosed metal particles, and amorphous carbon [13]. The density and growth rate of CNTs in Chemical vaporization Technique increase with an increase in temperature. Also, as the temperature increases, the CNTs tend to be vertically aligned. By using CVD, excellent alignment and positional control on the nanometer scale can be achieved in addition to controlling the diameter and the growth rate. A major drawback with the CVD technique is that there are high defect densities in the MWNT structures grown by this process. It is believed that it is most likely due to the lack of sufficient thermal energy for annealing CNTs because of relatively low growth temperature [13]. Usually the diameter of SWNT is in the range of 1.2 to 1.4 nm in arc discharge method [14], by using inert gas in arc discharge method the diameter is around 1.2 nm and using optical plasma control in arc discharge method the diameter is around 1.37 nm [16].

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But by using chemical vapour deposition the diameter of SWNT is in the range of 0.6 to 1.2 nm. If both electrodes are graphite in arc discharge method the main product will be Multi –Wall Nano Tubes. But next to MWNTs a lot of side products are formed such as fullerenes, amorphous carbon, and some graphite sheets. Purifying the MWNTs, means loss of structure and disorders the walls [15]. Typical sizes for MWNTs are an inner diameter of 1-3 nm and an outer diameter of approximately 10 nm. MWNT can be synthesized with low amount of defects in arc discharge method. Laser vaporization method results in a higher yield for SWNT synthesis and the nanotubes have better properties and a narrower size distribution than SWNTs produced by arc-discharge [15]. Nanotubes produced by laser ablation are purer (up to about 90 % purity) than those produced in the arc discharge process.

The different techniques for the Carbon nanotubes synthesis with CVD have been developed, such as plasma enhanced CVD, thermal chemical CVD, alcohol catalytic CVD, vapour phase growth, aero gel-supported CVD and laser-assisted CVD.[17][18][19][20]. The plasma enhanced CVD method generates a glow discharge in a chamber or a reaction furnace by a high frequency voltage applied to both electrodes. Figure 1 shows a schematic diagram of a typical plasma CVD apparatus with a parallel plate electrode structure.

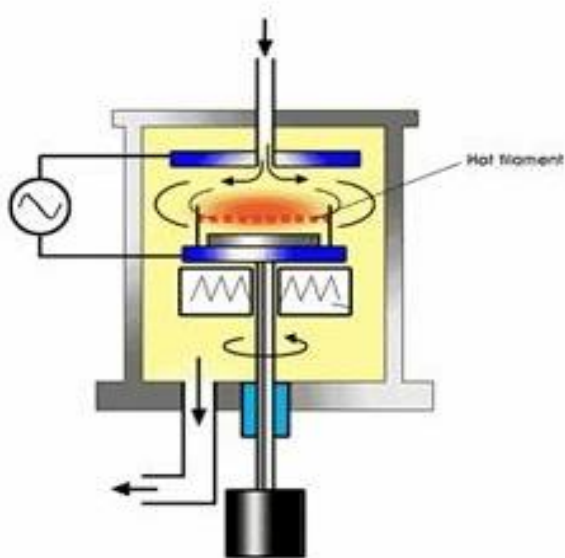


Figure 1: Schematic diagram of plasma CVD apparatus Taken from with permission. [15]

A substrate is placed on the grounded electrode. In order to form a uniform film, the reaction gas is supplied from the opposite plate. Catalytic metal, such as Fe, Ni and Co are used on for example a Si, SiO₂, or glass substrate using thermal CVD or sputtering. After nanoscopic fine metal particles are formed, carbon nanotubes will be grown on the metal particles on the substrate by glow discharge generated from high frequency power. The catalyst has a strong effect on the nanotube diameter, growth rate, wall thickness, morphology and microstructure. The diameter of the MWNTs is approximately 15 nm. The highest yield of carbon nanotubes achieved was about 50% and was obtained at relatively low temperatures (below 330^o C). When growing carbon nanotubes on a Fe catalytic film by thermal CVD, the diameter range of the Carbon nanotubes depends on the thickness of the catalytic film. By using a thickness of

13 nm, the diameter distribution lies between 30 and 40 nm. When a thickness of 27 nm is used, the diameter range is between 100 and 200 nm.

The carbon nanotubes formed are multiwalled Carbon nano tubes [21]. Vapour phase growth is another synthesis method of carbon nanotubes, directly supplying reaction gas and catalytic metal in the chamber without a substrate [22]. The diameter of the carbon nanotubes by using vapour phase growth is in the range of 2 – 4 nm for SWNTs [23] and between 70 and 100 nm for MWNTs [22]. In aero gel supported CVD method SWNTs are synthesized by disintegration of carbon monoxide on an aero gel-supported Fe/Mo catalyst. Because of the high surface area, the porosity and ultra-light density of the aero gels, the productivity of the catalyst is much higher than in other methods [24]. In laser-assisted thermal CVD (LCVD) a medium power, continuous wave CO₂ laser, which was Perpendicularly directed onto a substrate, pyrolyses sensitized mixtures of Fe (CO)₅ vapour and acetylene in a flow reactor. The carbon nanotubes are formed by the catalyzing action of the very small iron particles. By using a reactant gas mixture of iron pentacarbonyl vapour, ethylene and acetylene both single- and multi-walled carbon nanotubes are produced. Silica is used as substrate. The diameters of the SWNTs range from 0.7 to 2.5 nm. The diameter range of the MWNTs is 30 to 80 nm [25]. In comparing all three process PECVD has got typical yield of 20 to 100 % and also long tubes in μm with diameter of 0.6 to 4 m. Even MWNT of diameter 10 to 240 nm is possible in PECVD [15]. Only drawback is little bit structural defects in MWNT in PECVD process.

III CNT TYPES – STUDY OF ITS STRUCTURES

A single wall carbon nanotube can be described as a graphene sheet rolled into a cylindrical shape so that the structure is one-dimensional with axial symmetry [28] Nanotubes have caps on each end of the graphene sheets, which contain six pentagons. The caps are placed perfectly to fit the long cylindrical section. Carbon nanotubes are approximately a nanometer wide and a few microns long. The classifications of the different symmetries of nanotubes are dependent on the unit cell. The unit cell is a section of the carbon nanotube, which is broken down into vectors that describe the spiral symmetry of the nanotube. Nano tube structures are represented by the following parameters [29]

- 1) Chiral vector = $\mathbf{Ch} = n\mathbf{a}_1 + m\mathbf{a}_2 \equiv (n, m)$
 - 2).Translational vector = $\mathbf{T} = t_1\mathbf{a}_1 + t_2\mathbf{a}_2 \equiv (t_1, t_2)$
 - 3) Chiral angle = $\cos\theta = (2n + m) / (2\sqrt{n^2 + m^2 + n*m})$
 - 4) Length of chiral vector = $L = a\sqrt{n^2 + m^2 + n*m}$
Where a is the lattice constant
 - 5) Diameter = $d_t = L/\pi$
 - 6) Number of hexagons in the unit cell = $N = (2*(n^2 + m^2 + n*m))/dR$
 - 7) Symmetry vector = $\mathbf{R} = p\mathbf{a}_1 + q\mathbf{a}_2 \equiv (p, q)$
 - 8)Pitch of the symmetry vector = $\tau = ((m*p - n*q)*T)/N$
 - 9) Rotation angle of the symmetry vector = $\psi = 2\pi/N$ (in radians)
- where $t_1 = (2m + n)/dR$; $t_2 = -(2n + m)/dR$; $dR = \text{gcd}(2n+m, 2m+n)$, n,m are length of chiral vector.[28]



III.a..CNT ARM CHAIR TYPE

The symmetrical classification of an armchair nanotube is an achiral nanotube. Achiral means the nanotube has a structure that is a mirror image of the original one. An armchair nanotube has a chiral vector where $n = m$, therefore $\mathbf{Ch} = (n, n)$. The chiral angle θ is equal to 30° . For example, if $\mathbf{Ch} = (4, 4)$ the nanotube is an armchair nanotube where the chiral angle is equal to 30° . Table 1 shows the calculated parameters for armchair type carbon nano tube. Figure 2 a and b shows the armchair type [4,4] and [10,10] carbon nano tube simulated in nanotube modeler [30].

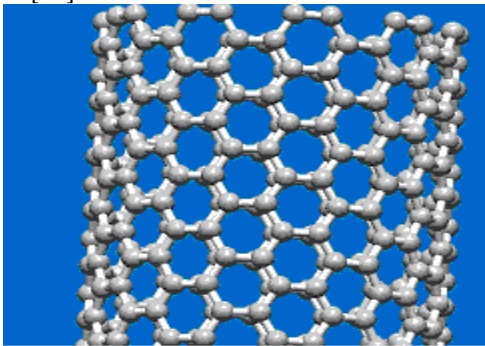


Figure 2.a shows SWCNT of chiral vector (10,10) of bond length 1.41 \AA and tube length 20 \AA . Courtesy Nano tube modeler / jcrystal.com

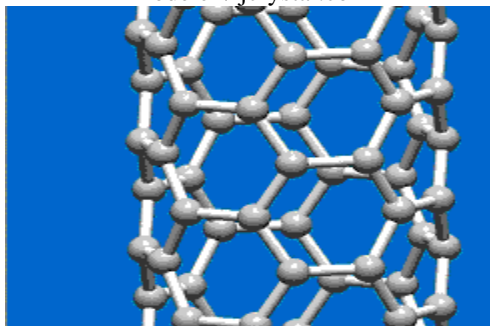


Figure 2.b shows SWCNT of chiral vector (4,4) of bond length 1.41 \AA and tube length 20 \AA . Courtesy Nano tube modeler / jcrystal.com

III.b. CNT ZIG ZAG TYPE

The symmetrical classification of a zigzag nanotube is an achiral nanotube, the same as an armchair nanotube. Achiral means the nanotube has a structure that is a mirror image of the original one, which is illustrated in Figure 3. A zigzag nanotube has a chiral vector where $m = 0$, therefore $\mathbf{Ch} = (n, 0)$. The chiral angle θ is equal to 0° . For example, if $\mathbf{Ch} = (10, 0)$ the nanotube is a zigzag nanotube where the chiral angle is equal to 0° . To verify that we can use the formula mentioned above and table 2 gives the calculation of above listed parameters for zigzag carbon nanotube. Figure 3 shows the Zigzag type of chiral vector (10,0) and has chiral angle always angle = 0° .

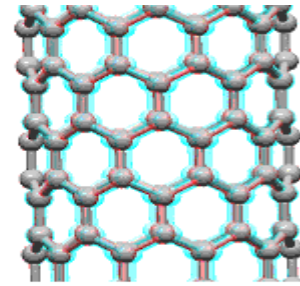


Figure 3 shows SWCNT of chiral vector (10,0) of bond length 1.41 \AA and tube length 20 \AA . Courtesy Nano tube modeler / jcrystal.com

III.c. CNT CHIRAL TYPE

The symmetrical classification of a chiral nanotube is a chiral nanotube. [29] Chiral means the nanotube has a spiral symmetry, which does not give it an identically structured mirror image. Figure 4 illustrates the structure of a chiral nanotube. A chiral nanotube has general n and m values, therefore $\mathbf{Ch} = (n, m)$. The chiral angle θ is between 0° and 30° , therefore $0^\circ < \theta < 30^\circ$. For example, if $\mathbf{Ch} = (4, 2)$ the nanotube is a chiral nanotube where the chiral angle is between 0° and 30° [29]. Table 3 gives calculated values for the chiral carbon nano tube parameters mentioned above.

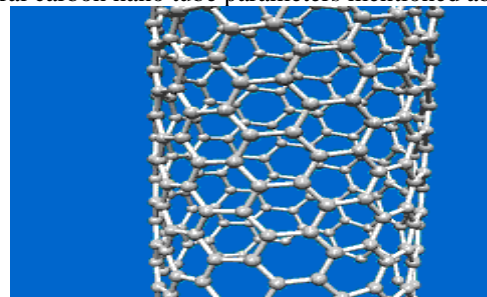


Figure 4 shows SWCNT of chiral vector (10,6) of bond length 1.41 \AA and tube length 20 \AA . Courtesy Nano tube modeler / jcrystal.com

III.d.CNT – DOUBLE WALLED AND MULTI WALLED TYPES

Double walled tube is constructed using Nano explorer and the separation between the sheets is around $d + 0.34 \text{ nm}$ [27] Where 'd' is the diameter of the inner tube. Figure 5 a and b shows the Double walled carbon nano tube and figure 6 a and b shows the Multiwalled carbon nano tube.

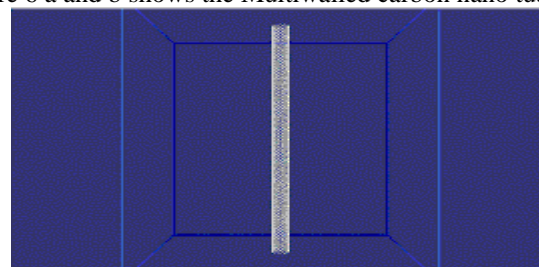


Figure 5 a double walled carbon nano tube from Nano explorer tool

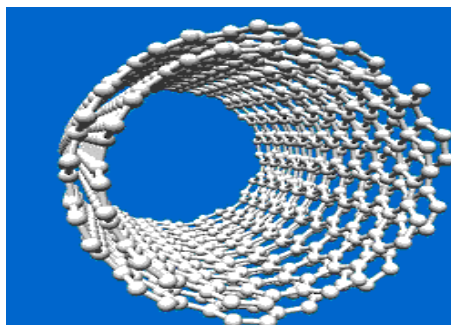


Figure 5 b shows double walled carbon nano tube with separation of $d + 0.34 \text{ nm}$ [27], length of CNT = 25 \AA . No of atoms = 894, No of bonds = 1297. Courtesy Nano tube modeler

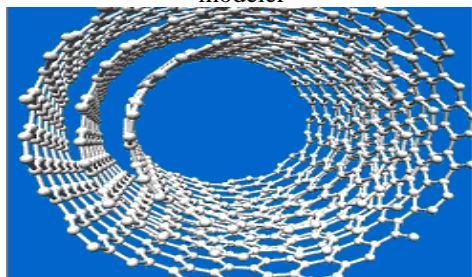


Figure 6 a Multi walled carbon nano tube without cap Courtesy Nano tube modeler front View, Armchair [10,10]

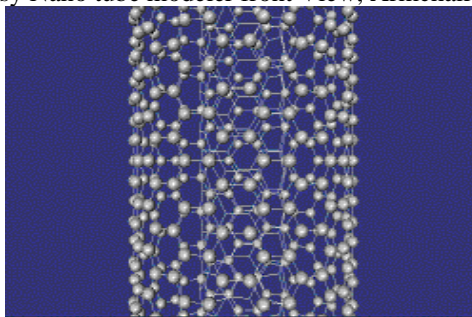


Figure 6 b Multi walled carbon nano tube without cap – side view Courtesy Nano explorer

III.e. CNT CAPPED TYPE – GRAPHENE SHEET.

All the above-simulated diagrams are without caps, Figure 7 a gives carbon nano tube with cap structure from Nano tube modeler. Figure 7 b gives graphite sheet generated using the simulation program written in Nano tube Modeller with height 15 \AA and width 20 \AA (No of rows and columns being 10). Figure 7 c gives graphite sheet of 260 atoms with 364 bonds using Nano tube modeler of armchair CNT (10,10)

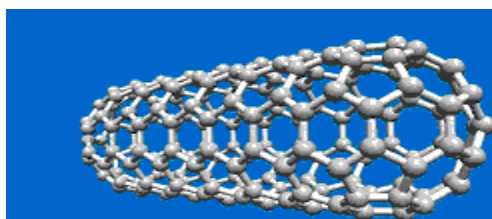


Figure 7 a capped carbon nano tube of armchair type [5,5] Courtesy Nano tube modeler.

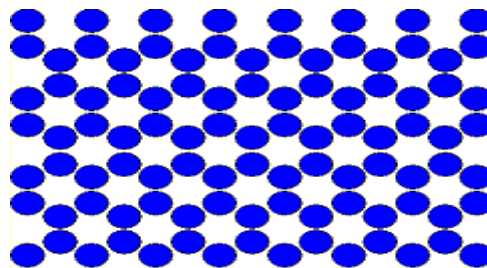


Figure 7 b is graphite sheet generated using Nano tube modeler

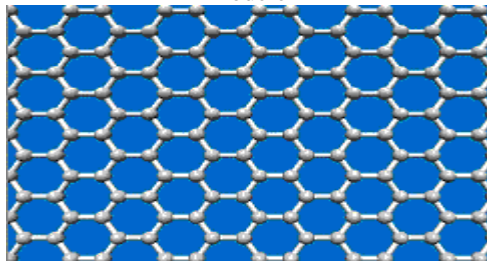


Figure 7 c is graphite sheet for arm chair carbon nano tube of [10,10] using nano tube modeler.

In this session we have simulated some of the basic structures of carbon nano tube using Nano explorer and Nano modeler, calculated and tabulated the structure parameters of three types of CNT and also generated simple graphite sheet of CNT.

VI CNT SIMULATIONS AND STRUCTURAL EFFECTS

Distortion in carbon nano tubes mainly depends on the properties of carbon nano tube, its synthesis and growth etc. Here we have simulated about the structural defects in carbon nano tube. There are mainly five basic important distortions

- 1.XY distortion
2. Z distortion
3. Twist
- 4.Bend
- 5.Deformation due to heterojunction

The XY and Z distortions are due to structural deformations may rise due to carbon nano tube synthesis and growth. [31][32]. When we measure the electrical and mechanical properties of the carbon nano tube through ATM and STM probe, the tip of the probe may also distort the structure of carbon nano tube. Figure 8 a, b, c, d shows the XY and Z distortion for (10,10) armchair carbon nano tube. The minimum deformation in XY plane and Z plane is measured to be 0.5 \AA .

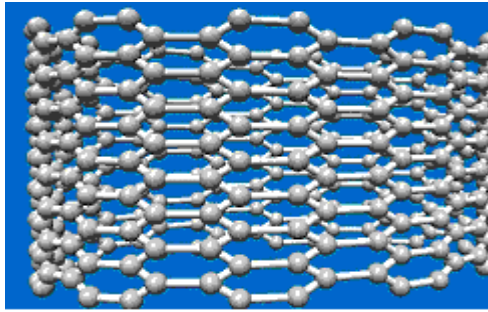


Figure 8 a Deformation in X-Y plane of (10,10) Armchair nanotube with length of tube 20 Å and Bond length 1.43 Å

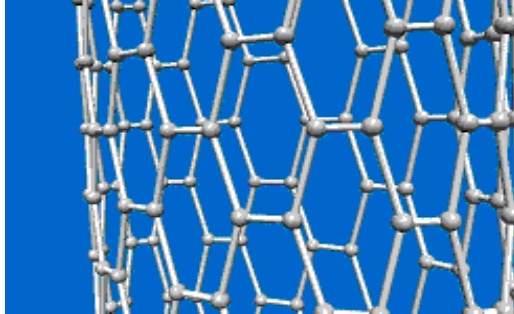


Figure 8 b Deformation in Z plane of (10,10) Armchair nanotube with length of tube 20 Å and Bond length 1.43 Å

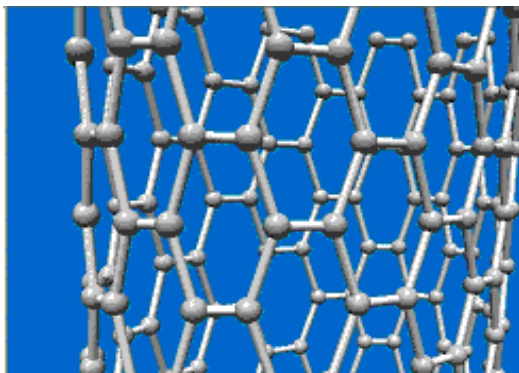


Figure 8 c Deformation due to both XY and Z plane- courtesy: Nano tube modeller

In figure 8c the deformation of Carbon nano tube on all directions are shown. Figure 8d and e shows the twist in angle of carbon nano tube and bend in length of carbon nano tube. Angle distortion in the simulation mainly due to lattice mismatch and structural deformations etc. We have shown angle twist of Armchair nano tube due to non-uniform arrangements of carbon atoms. The bend of the tube is due to increase in length of carbon nano tube as well as due to formation heterojunctions. If the twist is above 2° the more structural deformation takes place. Figure 8 e shows the bend in the length of the tube with angle of 2° and bend factor of 5. These type of tube distortions are simulated using nano tube modeler. These type are called basic types of nanotube distortions. This type of distortions arises due to the properties of CNT. These distortions are also useful in studying the structure of nano tube required for many applications.

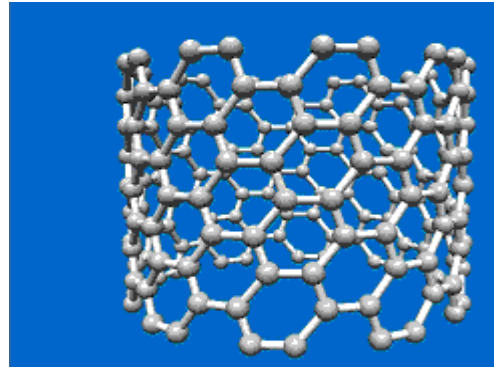


Figure 8 d shows the twist in angle of 2° Of Armchair Carbon nano tube [10,10] of length 20 nm – Courtesy Nano tube modeler.

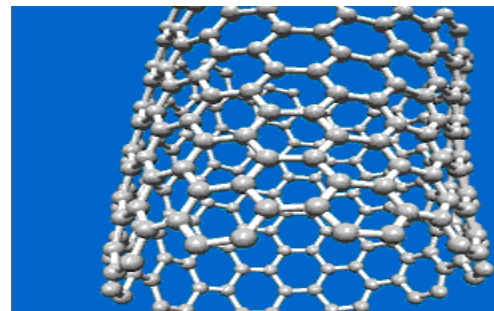


Figure 8 e shows the bend factor of 5 with angle 2° of armchair tube [10,10] Courtesy Nano tube modeler.

Now we will investigate about the metallic and semiconductor nature of some of the carbon nano tubes. It was stated that when the difference of integers n and m has divisible by 3 then the atoms behaves as metallic otherwise semi conducting [31][28]. Table 4 gives the metallic and semi conducting behavior of carbon nano tubes. It was proved from the table when $n-m$ is divisible by 3 then the behavior of tube is metallic otherwise semi conducting.

This session gives in details about the distortions occurring in the nano tube due to structure as well as angles. We also gave the electronic behavior of carbon nano tube as metals and semiconductor.

IV CNT PROPERTIES – STRUCUTRAL DEFECTS

IV.a CNT'S APPLICATIONS - Energy storage

Graphite, carbonaceous materials and carbon fibre electrodes are commonly used in fuel cells, batteries and other electrochemical applications. Advantages of considering nanotubes for energy storage are their small dimensions, smooth surface topology and perfect surface specificity. The efficiency of fuel cells is determined by the electron transfer rate at the carbon electrodes, which is the fastest on nanotubes following ideal Nernstian behaviour [32] The energy storage and medical applications of CNT are reviewed in this section and calculation of Energy per atom of CNT with respect its distance for storage applications are also plotted.

IV.a.1 HYDROGEN STORAGE

The advantage of hydrogen as energy source is that its combustion product is water. In addition, hydrogen can be easily regenerated. For this reason, a suitable hydrogen storage system is necessary, Satisfying a combination of both volume and weight limitations. The two commonly used means to store hydrogen are gas phase and electrochemical adsorption [15]. Because of their cylindrical and hollow geometry, and nanometer-scale diameters, it has been predicted that carbon nanotubes can store a liquid or a gas in the inner cores through a capillary effect.

The hydrogen storage requirements of 6.5 % by weight as the minimum level for hydrogen fuel cells. It is reported that SWNTs were able to meet and sometimes exceed this level by using gas phase adsorption (physisorption). Yet, most experimental reports of high storage capacities are rather controversial so that it is difficult to assess the applications potential. What lacks, is a detailed understanding of the hydrogen storage mechanism and the effect of materials processing on this mechanism. Another possibility for hydrogen storage is electrochemical storage. In this case not a hydrogen molecule but an H atom is adsorbed. This is called chemisorption. It was proved that hydrogen storage of 4 % even 6.5% of the weight storage is possible in CNT's [15]. We have calculated energy of an atom in CNT with respect to distance in A⁰ as per the given equation [15]

$$E_c = K a^2 / 24 \rho R^2 \quad 1.1$$

E_c be the energy per atom K.Cal / mol, a lattice constant, ρ be the density in gram / c.c R be the distance in A⁰. Table 5 gives the calculated energy for Zig Zag circular and non circular carbon nano tube. Figure 9 shows the energy per atom with respect R in A⁰. We found from the table 5 non-circular type CNT of atom has lesser energy than uniform circular type. We also calculated energy per atom for Zigzag, Armchair and chiral type CNT's and tabulated in table 6. Table 5 and 6 gives useful information about the hydrogen storage applications.

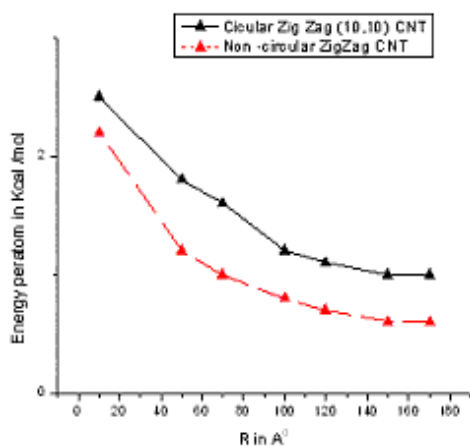


Figure 9 a shows plot of Energy per atom in CNT versus Radius (Distance).

Circular type CNT has energy storage maximum than over collapsed or elongated CNT's. As radius increases the energy decays and reaches constant value. The above

information useful for energy storage of hydrogen and lithium applications in CNT. We also calculated minimum Relative energy of atom in chiral tube CNT with respective to distance of no of iterations using Nanoexplorer tool by steepest descent method.

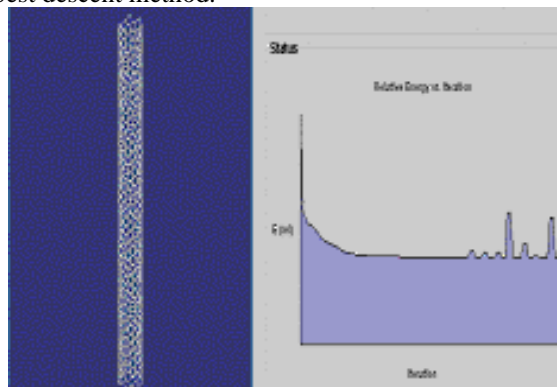


Figure 10 Chiral Carbon nano tube of relative energy calculations of atom Vs Radius.

IV.b CNT – MEDICAL APPLICATIONS
- CANCER CELL IDENTIFICATION

This paper attempts to report the existing and future applications of CNTs in the biomedical industry exclusively. We attempt to review the usage of CNT's particularly for cancer treatment. Then we report some of the properties [27] of CNT and simulated the structure for the given properties using Nano Explorer tool. A nanometer is a billionth of a meter. Nanotechnology is the creation of useful materials, devices, and systems through the manipulation of matter on this miniscule scale. Nanodevices being developed that have a potential to improve cancer detection, diagnosis, and treatment.

Nanomaterials have large surface areas relative to their volumes, phenomena like friction and sticking are more important than they are in larger systems. Nanostructures can be so small that the body may clear them too rapidly for them to be effective in detection or imaging. Larger nanoparticles may accumulate in vital organs, creating a toxicity problem.

Most animal cells are 10,000 to 20,000 nanometers in diameter. This means that nanoscale devices (less than 100 nanometers) can enter cells and the organelles inside them to interact with DNA and proteins. Tools developed through nanotechnology may be able to detect disease in a very small amount of cells or tissue. Detection of cancer at early stages is a critical step in improving cancer treatment. Currently, detection and diagnosis of cancer usually depend on changes in cells and tissues that are detected by a doctor's physical touch or imaging expertise. The potential for nanostructures to enter and analyze single cells suggests they could meet this need. [33].Figure 11 and 12 shows the nanodevices which are capable to enter the cell and also trace the structure of DNA to find any mutation on the DNA structure thereby identifying the cancerous cells



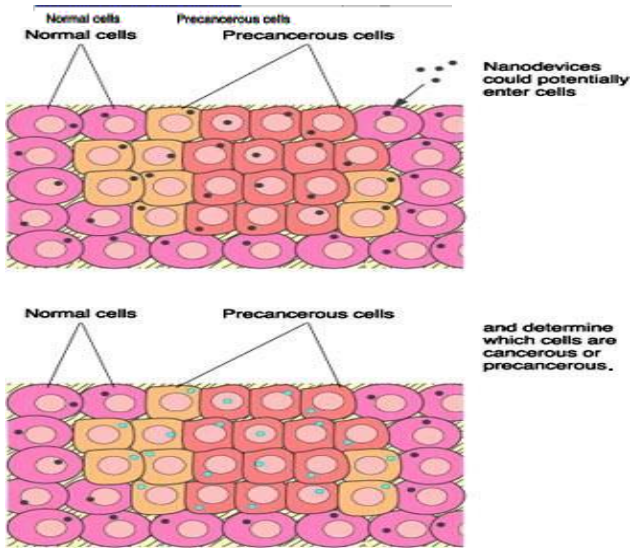


Figure 11 shows the size of nanodevice that can enter the human cell and to determine cancerous or precancerous cells [33]

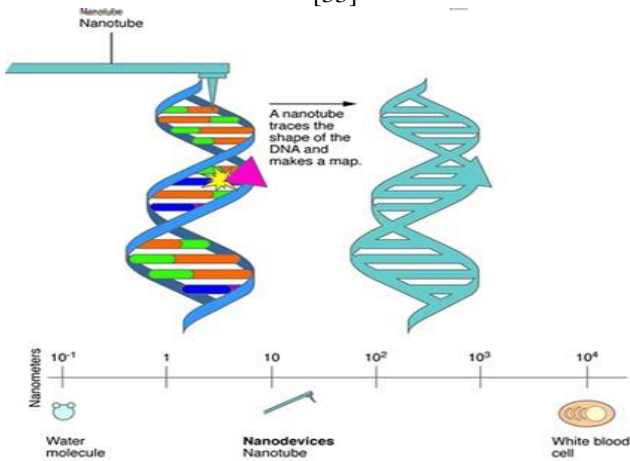


Figure 12 Carbon nano tube gliding over the surface of carbon nano tube to find the mutation on the surface.

Above diagram 11 and 12 shows nanodevice like carbon nano tube predicts and differentiates the cancerous cell with the ordinary cell [33].

IV.c CNT PHYSICAL AND CHEMICAL PROPERTIES

The properties of CNT are important because of miniature size. These properties tend to change as size, angle, and chiral vector of CNT's changes. We have taken some physical, electrical and mechanical properties from reference [27]. We simulated the CNT structure for above mentioned properties using Nanoexplorer tool.

V –CNT PROPERTIES

1. Given Chiral vector ex (10,10) Armchair tube, Diameter of tube 1.2nm, Carbon bond length – 1.42 Å, Overlap energy 2.5 eV, Lattice constant - 17 Å, density – 1.40 g/cm³, spacing between atoms 3.39 Å
2. Thermal Conductance – 1/12.9 kW⁻¹
3. Resistivity – 10⁻⁴ W - cm at 300°K
4. Conductivity – 10⁷ A / cm²

5. Young's modulus – 1 Tpa, Tensile strength – 30 gpa (yu etal)
6. Carbon bond length – 1.42 Å, overlap energy – 2.5eV, Lattice constant
7. Thermal conductivity – 1800 – 6000 w/m-k, carrier lifetime – 10e-11 sec. Figure 13 a and b shows the simulated structure for the above-mentioned properties of Zigzag (10,0) CNT. Figure 14 a and b shows the armchair type of CNT with above mentioned properties.

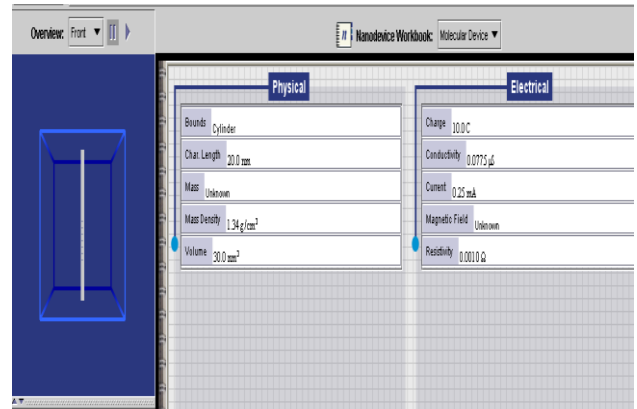


Figure 13 a shows the properties with the structure of Zig Zag CNT.

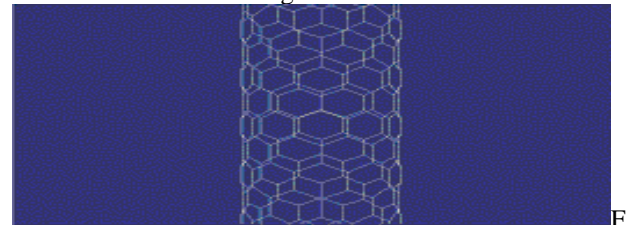


Figure 13 b shows the structure of (10,0) CNT. Courtesy Nanoexplorer tool

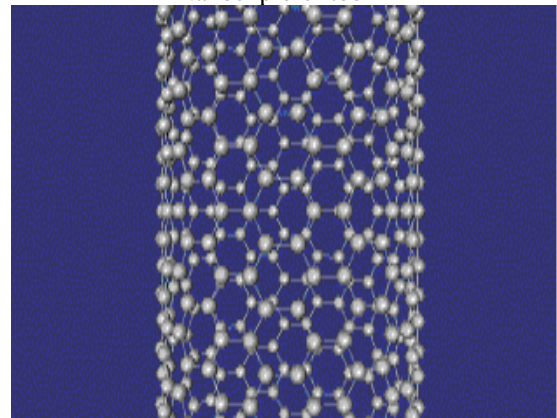


Figure 14 shows the (10,10) armchair type of CNT from Nanoexplorer

VI. Conclusion:

This paper describes the review of synthesis of carbon nano tube. It describes about the advantage of plasma enhanced CVD technique. Then we described about the simulation of CNT structures. We have calculated the structural parameters of types of CNT's.

The we mentioned about the various tube distortion in CNT and calculated energy per atom with respect to radius. We reviewed two important applications of CNT and finally some of the properties of CNT being mentioned and simulated the structure according to the structure.

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Table 1 Arm chair type Carbon nano tube structure parameters calculated using nanotube modeler with length of the tube 25 A⁰ and bond length 1.43 A⁰

s.no	Chiral vector	Chiral angle	Translational vector (degrees)	Length of chiral vector (A ⁰)	Diameter (A ⁰)	No of Hexagons in unit cell	No of atoms in CNT	NO of bonds used in CNT
1	4,4	30 ⁰	1, -1	9.9	3.152866	8	136	196
2	5,5	30 ⁰	1, -1	12.38	12.38	10	175	245
3	6,6	30 ⁰	1, -1	14.85	4.729299	12	204	294
4	7,7	30 ⁰	1, -1	17.33	5.519108	14	238	343
5	8,8	30 ⁰	1, -1	19.8	6.305732	16	272	392
6	9,9	30 ⁰	1, -1	22.28	7.095541	18	306	441
7	10,10	30 ⁰	1, -1	24.76	7.88535	20	340	490
8	11,11	30 ⁰	1, -1	27.23	8.658188	22	462	671
9	12,12	30 ⁰	1, -1	29.71	9.461783	24	504	732
10	13,13	30 ⁰	1, -1	32.18	10.24841	26	546	793
11	14,14	30 ⁰	1, -1	34.66	11.03822	28	588	854
12	15,15	30 ⁰	1, -1	37.14	11.82803	30	630	915
13	16,16	30 ⁰	1, -1	39.61	12.61465	32	672	976
14	17,17	30 ⁰	1, -1	42.09	13.40446	34	714	1037
15	18,18	30 ⁰	1, -1	44.56	14.19108	36	756	1098
16	19,19	30 ⁰	1, -1	47.044	14.98217	38	798	1159
17	20,20	30 ⁰	1, -1	49.52	15.7707	40	840	1220
18	21,21	30 ⁰	1, -1	51.99	16.55732	42	882	1281
19	22,22	30 ⁰	1, -1	54.47	17.34713	44	928	1342
20	23,23	30 ⁰	1, -1	56.94	1.813376	46	966	1403
21	24,24	30 ⁰	1, -1	59.42	18.92357	48	1008	1464



Table 2 Zigzag type of Carbon nano tube structure parameters calculated using nanotube modeler with length of the tube 25 Å⁰ and bond length 1.43 Å⁰

s.no	Chiral vector	Chiral angle (degrees)	Translational vector	Length of chiral vector (nm)	Diameter (nm)	No of Hexagons in unit cell	No of atoms in CNT	NO of bonds used in CNT
1	6,0	0 ⁰	1, -2	8.58	2.732	12	144	204
2	7,0	0 ⁰	1, -2	10.01	3.144	14	168	238
3	8,0	0 ⁰	1, -2	11.44	3.643	16	192	272
4	9,0	0 ⁰	1, -2	12.87	4.098	18	216	306
5	10,0	0 ⁰	1, -2	14.3	4.554	20	240	340
6	11,0	0 ⁰	1, -2	15.73	5.009	22	264	374
7	12,0	0 ⁰	1, -2	17.16	5.46	24	288	408
8	13,0	0 ⁰	1, -2	18.59	5.92	26	312	442
9	14,0	0 ⁰	1, -2	20.02	6.375	28	336	476
10	15,0	0 ⁰	1, -2	21.45	6.83	30	360	510
11	16,0	0 ⁰	1, -2	22.88	7.286	32	384	544
12	17,0	0 ⁰	1, -2	24.31	7.74	34	408	578
13	18,0	0 ⁰	1, -2	25.74	8.19	36	432	612
14	19,0	0 ⁰	1, -2	27.27	8.65	38	456	646
15	20,0	0 ⁰	1, -2	28.6	9.108	40	480	680
16	21,0	0 ⁰	1, -2	30.03	9.56	42	504	714
17	22,0	0 ⁰	1, -2	31.46	10.019	44	528	748
18	23,0	0 ⁰	1, -2	32.84	10.458	46	552	782
19	24,0	0 ⁰	1, -2	34.32	10.92	48	576	816
20	25,0	0 ⁰	1, -2	37.75	11.38	50	600	850

Table 3 Zigzag type of Carbon nano tube structure parameters calculated using nanotube modeler with length of the tube 25 Å⁰ and bond length 1.43 Å⁰

s.no	Chiral vector	Chiral angle (degrees)	Translational vector	No of atoms in CNT	NO of bonds used in CNT
1	4,2	19 ⁰	4,-5	126	182
2	10,6	21.78 ⁰	11,-13	332	480
3	12,8	23.14 ⁰	7,-8	412	596
4	15,12	26.32 ⁰	12,-14	555	804
5	18,16	28.02 ⁰	25,-26	642	1012

Table 4 Electronic behavior of atom in chiral carbon nano tube

S.NO	Chiral vector of Chiral CNT (nm)	Diameter of tube (nm)	Chiral angle (Degree)	Electronic behavior
1	13,3	1.15	19.8	Semi conductor
2	14,2	1.18	23.4	Metal
3	13,4	1.21	17	Metal
4	14,3	1.23	20.5	Semiconductor
5	15,2	1.26	23.8	Semiconductor
6	14,4	1.28	17.8	Semiconductor
7	15,3	1.31	21.1	Metal

Table 5 Energy calculation of atom in CNT of circular and non-circular with radius(distance) R

S.NO	Radius (Distance) in A ⁰	Energy of circular CNT (Zig Zag) K.cal / Mol	Energy of non - circular CNT (Zig Zag) K.cal / Mol
1	10	2.5	2.2
2	50	1.8	1.2
3	70	1.6	1.0
4	100	1.2	0.8
5	120	1.1	0.7
6	150	1.0	0.6
7	170	1.0	0.6

Table 6 Energy of circular and non-circular of three types of CNT. No of atoms taken be 50.

S.NO	Type of CNT	Radius in A ⁰	Energy of circular CNT (K.Cal / Mol)	Energy of non –circular CNT – (K.Cal /Mol)
1	Armchair (12,12)	7.5	2.89	2.17
2	Zig Zag (15,0)	4.89	3.83	2.8
3	Chiral (14,7)	14.8	2.2	1.6