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Three-Dimensional Finite Element (FE) Model for Armchair and Zigzag Type Single-Walled Carbon Nanotubes

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***Abstract*-** Three-dimensional finite element (FE) model for armchair and zigzag type single-walled carbon nanotubes (SWCNTs) is proposed. The model development is based on the assumption that carbon nanotubes, when subjected to loading, behave like space-frame structures. The bonds between carbon atoms are considered as connecting load-carrying members, while the carbon atoms as joints of the members. To create the FE models, nodes are placed at the locations of carbon atoms and the bonds between them are modeled using three-dimensional shell element. The elastic moduli of shell element is determined by using a linkage between molecular and continuum mechanics. The investigation includes armchair and zigzag SWCNTs.

It is found that the choice of Vander wall forces, the interaction significantly affects the calculation of Young's modulus. The obtained values of Young's modulus agree very well with the corresponding theoretical results and many experimental measurements. Dependence of elastic moduli to diameter and length of the nanotubes is also obtained. The presented results demonstrate that the proposed FE model may provide a valuable tool for studying the mechanical behavior of carbon nanotubes and their integration in nano composites.

So far we dealt with single walled carbon nanotube. The elements were considered as shell element, it is a uniaxial element with tension, compression, torsion, and bending capabilities. The element has six degrees of freedom at each node: translations in the nodal x, y, and z directions and rotations about the nodal x, y, and z axes. Stress stiffening and large deflection capabilities are included.

I. INTRODUCTION

Nanotubes are members of the fullerene structural family. Their name is derived from their long, hollow structure with the walls formed by one-atom-thick sheets of carbon, called graphene. These sheets are rolled at specific and discrete angles, and the combination of the rolling angle and radius decides the Nanotube properties. Within the layers the atoms are arranged at the corners of hexagons which fill the whole plane. The carbon atoms are strongly (covalently) bound to each other (carbon-carbon distance ~ 0.14 nm). The layers themselves are rather weakly bound to each other.

Carbon nanotubes (CNTs) are amongst the mostexplored one-dimensional nanostructures and have attracted tremendous interest from fundamental science and technological perspectives. CNTs have been used in many laboratories to build prototype nanodevices. These devices include metallic wires, field-effect transistors, electromechanical sensors and displays. They potentially form the basis of future all-carbon electronics.

A carbon nanotube can be considered as a large molecule consisting of carbon atoms, forming a hexagonal mesh. It may also be regarded as a one atom thick sheet of graphite, rolled into a tube with high aspect ratio. Such a tube can be considered as a fundamental structural unit, known as single-walled carbon nanotube. Using that fundamental structural unit, a multi-walled carbon nanotube can be formed. MWNTs are in fact concentrically nested SWNTs, with a distance between the layers or walls equal to 0.34 nm.

Each atom in a single layer has three nearest neighboring atoms and they are bonded by covalent bonds, which have characteristic properties (bond length and bond angle). Atoms on different layers of MWNTs are not connected by covalent bonds and the only interaction between them is through Vander Waals forces. Vander Waals forces are rather weak compared to covalent bonds.

Carbon nano tubes are held together by means of strong sp2 covalent bonding between carbon atoms. The weak interlayer coupling gives graphite the property of a seemingly very soft material. One of the physical properties of carbon nanotubes is that it's possible to make them only a single atomic layer thick. This means that they can be about 1/50,000th the thickness of a human hair

1.1 BACKGROUND LEADING UP TO CARBON NANOTUBES

Until the mid-1980's pure solid carbon was thought to exist in only two physical forms, diamond and graphite. Diamond and graphite have different physical structures and properties however their atoms are both arranged in covalently bonded networks. These two different physical forms of carbon atoms are called allotropes.

In 1985 a group of researchers led by Richard Smalley and Robert Curl of Rice University in Houston and Harry Kroto of the University of Sussex in England made an interesting discovery. They vaporized a sample of graphite with an intense pulse of laser light and used a stream of helium gas to carry the vaporized carbon into a mass spectrometer.

The mass spectrum showed peaks corresponding to clusters of carbon atoms, with a particularly strong peak corresponding to molecules composed of 60 carbon atoms, C60. The fact that C 60 clusters were so easily formed led the group to propose that a new form or allotrope of carbon had been discovered. It was spherical in shape and formed a ball with 32 faces. Of the 32

faces, 12 were pentagons and 20 were hexagons exactly like a soccer ball.(as shown in fig below)

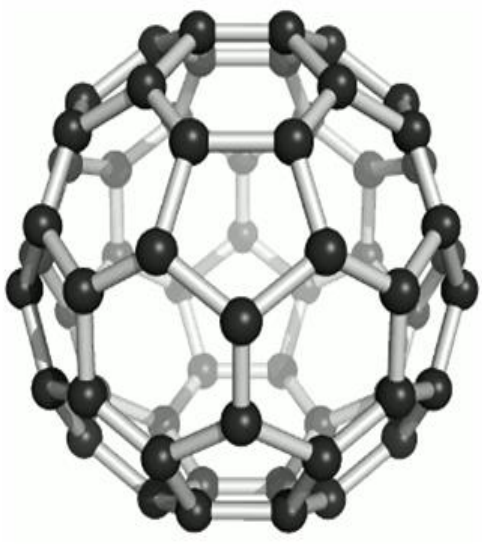

Fig.1 Buckminster fullerene

We see this unusual soccer ball-shape expressed in a wide variety of physical objects, for instance soccer balls, new golf balls, architecture, and art. These molecules were named after an architect, Buckminster Fuller, who was responsible for the design of the first geodomes. A geodome that you may be familiar with is "Spaceship Earth" at Epcot Center (Disney World). The soccer ball shaped C60 molecule was named “Buckminster Fullerene” or “buckyball” for short.

After this discovery, other related molecules (C36, C70, C76 and C84) composed of only carbon atoms were also discovered and they and the buckyball were recognized as a new allotrope of carbon. This new class of carbon molecules is called the fullerenes. Fullerenes consist of hexagons and pentagons that form a spherical shape. Fullerenes have also been proposed as possible HIV inhibitors as well as potential constituents in interstellar space.

1.2 DISCOVERY OF CARBON NANOTUBES

The unique geometric properties of this new allotrope of carbon did not end with soccer shaped molecules, it was also discovered that carbon atoms can form long cylindrical tubes. These tubes were originally called “buckytubes” but now are better known as carbon nanotubes or CNT for short. These molecules are shaped like a tube; imagine a sheet of graphite ("graphene sheet") or chicken wire rolled into a tube.

The carbon Nanotube was discovered in 1991 by the Japanese electron microscopist Sumio Iijima who was studying the material deposited on the cathode during the arc-evaporation synthesis of fullerenes. He found that the central core of the cathodic deposit contained a variety of closed graphitic structures including nanoparticles and nanotubes, of a type which had never previously been observed.

The tubes are hollow cylinders with diameters ranging from 1 to 50 nm and having a length in the range of micrometers. Nanotubes have been constructed with length-to-diameter ratio of up to 132,000,000:1, significantly larger than for any other material. The properties of the material vary as the surface to volume ratio varies. **They only contain carbon atoms and can be thought of a seamless cylinder rolled from a graphite sheet.** Extensive experiments using various advanced measurement tools have been carried out to identify the mechanical properties and the behaviors of CNT including the Young’s modulus, shear modulus, buckling behavior and vibration responses. Due to their exceptional mechanical and electrical properties: small size, low density, high stiffness, high strength etc., CNTs represent a very promising material in many areas of science and industry.

Carbon Nanotubes have many structures, differing in length, thickness, and in the type of helicity and number of layers. Although they are formed from essentially the same graphite sheet, their electrical characteristics differ depending on these variations, acting either as metals or as semiconductors.

1.3.Classification of carbon nano tubes

Carbon Nanotubes can be classified mainly based on the following two factors

1.3.1 Classification based on chirality

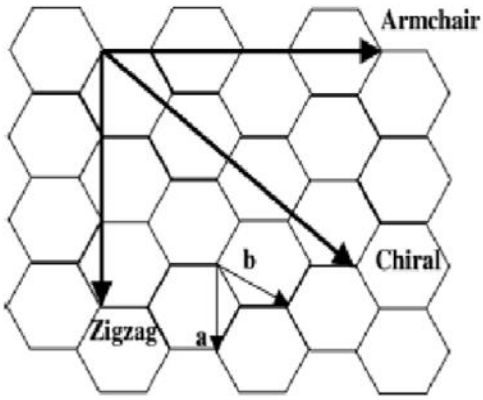

Fig.2 representation of chirality of CNT

The way the graphene sheet is wrapped is represented by a pair of indices (n, m). The integer’s n and m denote the number of unit vectors along two directions in the honeycomb crystal lattice of graphene. If m = 0, the nanotubes are called **zigzag nanotubes**, and if n = m, the nanotubes are called **armchair nanotubes**. Otherwise, they are called **Chiral.** The diameter of an ideal Nanotube can be calculated from its (n, m) indices as follows

$$d = \frac{a}{\pi}\sqrt{(n^2 + nm + m^2)}.$$

where a = 0.246 nm.

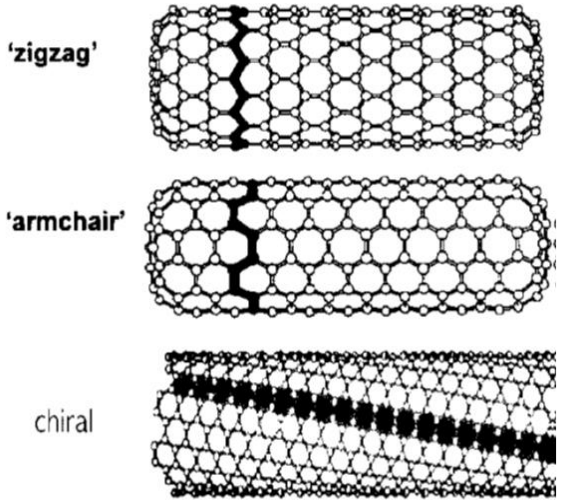

Fig.3 Armchair, Zigzag and Chiral CNTS

Our current project deals about comparison between the armchair and zigzag type of tubes at different wall thickness and at different loading conditions.

1.3.2 Based on number of graphene sheets being rolled

Single walled carbon nano tubes (SWNT**)** are most widely used nano tubes. Most single-walled nanotubes have a diameter of close to 1 nanometer, with a tube length that can be many millions of times longer. The structure of a SWNT can be conceptualized by wrapping a one-atom-thick layer of graphite called graphene into a seamless cylinder. Single-walled nanotubes are likely candidates for miniaturizing electronics. The most basic building block of these systems is the electric wire, and SWNTs with diameters of an order of a nanometer can be excellent conductors. One useful application of SWNTs is in the development of the first intermolecular field-effect transistors.

Multi-walled carbon nanotubes (MWNT) consist of multiple rolled layers (concentric tubes) of graphene. There are two models that can be used to describe the structures of multi-walled nanotubes. In the Russian Doll model, sheets of graphite are arranged in concentric cylinders. In the Parchment model, a single sheet of graphite is rolled in around itself, resembling a scroll of parchment or a rolled newspaper The interlayer distance in multi-walled nanotubes is close to the distance between graphene layers in graphite, approximately 3.4 Å. Multi walled carbon nano tubes are mainly used in space elevators due to their extreme physical properties.

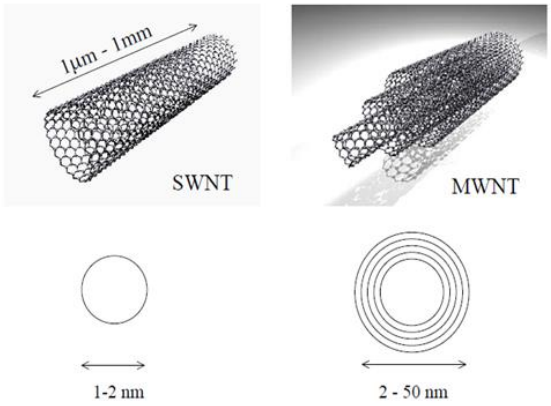

Fig.4 Single wall / Multi wall nanotubes

The failure criteria of CNTS are described by its compressive loading condition. Carbon nano tubes mainly fail due to buckling. Buckling is characterized by a sudden failure of a structural member subjected to high compressive stress, where the actual compressive stress at the point of failure is less than the ultimate compressive stresses that the material is capable of withstanding.

1.4. PROPERTIES OF CARBON NANO TUBES

Carbon nano tubes are quite interesting than the other nano materials because of their excellent properties that they can exhibit. Some of the properties that a carbon nano tube can exhibit are clearly discussed in this paper. The properties of the carbon nano tubes will not be the same for each and every tube. There will be a significant change in properties as the length to diameter ratio varies.

1.4.1. MECHANICAL PROPERTIES

Carbon nanotube is one of the strongest materials in nature. Carbon nanotubes (CNTs) are basically long hollow cylinders of graphite sheets. Although a graphite sheet has a 2D symmetry, carbon nanotubes by geometry have different properties in axial and radial directions. It has been shown that CNTs are very strong in the axial direction. Young's modulus on the order of270 - 950 GPA and tensile strength of 11 - 63 GPA were obtained.

On the other hand, there was evidence that in the radial direction they are rather soft. The first transmission electron microscope observation of radial elasticity suggested that even the van der Waals forces can deform two adjacent nanotubes. Later, nano indentations with atomic force microscope were performed by several groups to quantitatively measure radial elasticity of multiwalled carbon nanotubes and tapping/contact mode atomic force microscopy was recently performed on single-walled carbon nanotubes. Young's modulus of on the order of several GPA showed that CNTs are in fact very soft in the radial direction.

Radial direction elasticity of CNTs is important especially for carbon nanotube composites where the embedded tubes are subjected to large deformation in the transverse direction under the applied load on the composite structure.

1.4.2. Strength

Carbon nanotubes are the strongest and stiffest materials yet discovered in terms of tensile strength and elastic modulus respectively. This strength results from the covalent sp^2 bonds formed between the individual carbon atoms. CNTs are not nearly as strong under compression. Because of their hollow structure and high aspect ratio, they tend to undergo buckling when placed under compressive, torsional, or bending stress.

Further studies, such as one conducted in 2008, revealed that individual CNT shells have strengths of up to ~100 GPa, which is in agreement with quantum/atomistic models. Since carbon nanotubes have a low density for a solid of 1.3 to 1.4 g/cm^3, its specific strength of up to 48,000 kN·m·kg^{-1} is the best of known materials, compared to high-carbon steel's 154 kN·m·kg^{-1}. Under excessive tensile strain, the tubes will undergo plastic deformation, which means the deformation is permanent.

Although the strength of individual CNT shells is extremely high, weak shear interactions between adjacent shells and tubes leads to significant reductions in the effective strength of multi-walled carbon nanotubes and carbon nanotube bundles down to only a few GPa's.

1.4.3. Hardness

Standard single-walled carbon nanotubes can withstand a pressure up to 24 GPA without deformation. They then undergo a transformation to super hard phase nanotubes. Maximum pressures measured using current experimental techniques are around 55 GPA. However, these new super hard phase nanotubes collapse at an even higher, unknown, pressure. The bulk modulus of super hard phase nanotubes is 462 to 546 GPA, even higher than that of diamond (420 GPA for single diamond crystal).

1.4.4. Kinetic properties

Multi-walled nanotubes are multiple concentric nanotubes precisely nested within one another. These exhibit a striking telescoping property whereby an inner nanotube core may slide, almost without friction, within its outer nanotube shell, thus creating an atomically perfect linear or rotational bearing. This is one of the first true examples of molecular nanotechnology, the precise positioning of atoms to create useful machines. Already, this property has been utilized to create the world's smallest rotational motor. Future applications such as a gigahertz mechanical oscillator are also envisaged.

1.4.5. Electrical properties

Because of the symmetry and unique electronic structure of graphene, the structure of a nanotube strongly affects its electrical properties. For a given (n, m) nanotube, if $n = m$, the nanotube is metallic; if $n - m$ is a multiple of 3, then the nanotube is semiconducting with a very small band gap, otherwise the nanotube is a moderate semiconductor. Thus all armchair ($n = m$) nanotubes are metallic, and nanotubes (6, 4), (9, 1), etc. are semiconducting.

Because of their nanoscale cross-section, electrons propagate only along the tube's axis and electron transport involves quantum effects. As a result, carbon nanotubes are frequently referred to as one-dimensional conductors. There have been reports of intrinsic superconductivity in carbon nanotubes. Many other experiments, however, found no evidence of superconductivity, and the validity of these claims of intrinsic superconductivity remains a subject of debate.

1.4.6. Optical Properties

Within materials science, the optical properties of carbon nanotubes refer specifically to the absorption, photoluminescence, and Raman spectroscopy of carbon nanotubes. Spectroscopic methods offer the possibility of quick and non-destructive characterization of relatively large amounts of carbon nanotubes. There is a strong demand for such characterization from the industrial point of view: numerous parameters of the nanotube synthesis can be changed, intentionally or unintentionally, to alter the nanotube quality.

Carbon nanotubes are unique "one dimensional systems" which can be envisioned as rolled single sheets of graphite (or more precisely graphene). This rolling can be done at different angles and curvatures resulting in different nanotube properties. The diameter typically varies in the range 0.4–40 nm (i.e. "only" ~100 times), but the length can vary ~10,000 times reaching 18.5 cm. Thus the nanotube aspect ratio, or the length-to-diameter ratio, can be as high as 132,000,000:1, which is unequalled by any other material. Consequently, all the properties of the carbon nanotubes relative to those of typical semiconductors are extremely anisotropic (directionally dependent) and tunable.

1.4.7. Thermal properties

As nanoscale graphitic structures, carbon nanotubes are of great interest for their thermal properties. The low-temperature specific heat and thermal conductivity show direct evidence of 1-D quantization of the phonon band structure. Modeling of the low-temperature specific heat allows determination of the on-tube phonon velocity, the splitting of phonon sub bands on a single tube, and the interaction between neighboring tubes in a bundle.

All nanotubes are expected to be very good thermal conductors along the tube, exhibiting a property known as "ballistic conduction", but good insulators laterally to the tube axis. Measurements show that a SWNT has a room-temperature thermal conductivity along its axis of about 3500 W·m^{-1}·K^{-1}; compare this to copper, a metal well known for its good thermal conductivity, which transmits 385 W·m^{-1}·K^{-1}. A SWNT has a room-temperature thermal conductivity across its axis (in the radial direction) of about 1.52 W·m^{-1}·K^{-1}, which is about as thermally conductive as soil. The temperature stability of carbon nanotubes is estimated to be up to 2800 °C in vacuum and about 750 °C in air.

1.5. Applications of Carbon nano tubes

1.5.1. Current Applications

Current use and application of nanotubes has mostly been limited to the use of bulk nanotubes, which is a mass of rather unorganized fragments of nanotubes. Bulk nanotube materials may never achieve a tensile strength similar to that of individual tubes, but such composites may, nevertheless, yield strengths

sufficient for many applications. Bulk carbon nanotubes have already been used as composite fibers in polymers to improve the mechanical, thermal and electrical properties of the bulk product.

1.5.2. Potential Applications

The strength and flexibility of carbon nanotubes makes them of potential use in controlling other nanoscale structures, which suggests they will have an important role in nanotechnology engineering. The highest tensile strength of an individual multi-walled carbon nanotube has been tested to be is 63 GPa. Carbon nanotubes were found in Damascus steel from the 17th century, possibly helping to account for the legendary strength of the swords made of it.

1.5.3. Structural

Because of the carbon nanotubes superior mechanical properties, many structures have been proposed ranging from everyday items like clothes and sports gear to combat jackets and space elevators. However, the space elevator will require further efforts in refining carbon nanotube technology, as the practical tensile strength of carbon nanotubes can still be greatly improved.

Carbon nanotubes are also a promising material as building blocks in bio-mimetic hierarchical composite materials given their exceptional mechanical properties (~1 TPa in modulus, and ~100 GPa in strength). Initial attempts to incorporate CNTs into hierarchical structures led to mechanical properties that were significantly lower than these achievable limits. Because of the high mechanical strength of carbon nanotubes, research is being made into weaving them into clothes to create stab-proof and bulletproof clothing. The nanotubes would effectively stop the bullet from penetrating the body, although the bullet's kinetic energy would likely cause broken bones and internal bleeding.

1.5.4. In electrical circuits

Nanotube-based transistors, also known as carbon nanotube field-effect transistors (CNTFETs), have been made that operate at room temperature and that are capable of digital switching using a single electron. However, one major obstacle to realization of nanotubes has been the lack of technology for mass production. In 2001 IBM researchers demonstrated how metallic nanotubes can be destroyed, leaving semiconducting ones behind for use as transistors. Their process is called "constructive destruction," which includes the automatic destruction of defective nanotubes on the wafer. This process, however, only gives control over the electrical properties on a statistical scale.

1.5.5. As electrical cables and wires

Wires for carrying electrical current may be fabricated from pure nanotubes and nanotube-polymer composites. Recently small wires have been fabricated with specific conductivity exceeding copper and aluminum; these cables are the highest conductivity carbon nanotube and also highest conductivity non-metal cables.

1.5.6. As paper batteries: A paper battery is a battery engineered to use a paper-thin sheet of cellulose (which is the major constituent of regular paper, among other things) infused with aligned carbon nanotubes. The nanotubes act as electrodes; allowing the storage devices to conduct electricity. The battery, which functions as both a lithium-ion battery and a super capacitor, can provide a long, steady power output comparable to a conventional battery, as well as a super capacitor's quick burst of high energy—and while a conventional battery contains a number of separate components, the paper battery integrates all of the battery components in a single structure, making it more energy efficient.

1.5.7. Solar cells

One of the promising applications of single-walled carbon nanotubes (SWNTs) is their use in solar panels, due to their strong UV/Vis-NIR absorption characteristics. Research has shown that they can provide a sizeable increase in efficiency, even at their current un-optimized state. Solar cells developed at the New Jersey Institute of Technology use a carbon nanotube complex, formed by a mixture of carbon nanotubes and carbon buckyballs (known as fullerenes) to form snake-like structures. Buckyballs trap electrons, but they can't make electrons flow. Add sunlight to excite the polymers, and the buckyballs will grab the electrons. Nanotubes, behaving like copper wires, will then be able to make the electrons or current flow.

1.5.8. Hydrogen storage

In addition to being able to store electrical energy, there has been some research in using carbon nanotubes to store hydrogen to be used as a fuel source. By taking advantage of the capillary effects of the small carbon nanotubes, it is possible to condense gases in high density inside single-walled nanotubes. This allows for gases, most notably hydrogen (H_2), to be stored at high densities without being condensed into a liquid. Potentially, this storage method could be used on vehicles in place of gas fuel tanks for a hydrogen-powered car. A current issue regarding hydrogen-powered vehicles is the onboard storage of the fuel. Current storage methods involve cooling and condensing the H_2 gas to a liquid state for storage which causes a loss of potential energy (25–45%) when compared to the energy associated with the gaseous state. Storage using SWNTs would allow one to keep the H2 in its gaseous state, thereby increasing the storage efficiency. This method allows for a volume to energy ratio slightly smaller to that of current gas powered vehicles, allowing for a slightly lower but comparable range.

An area of controversy and frequent experimentation regarding the storage of hydrogen by adsorption in carbon nanotubes is the efficiency by which this process occurs. The effectiveness of hydrogen storage is integral to its use as a primary fuel source since hydrogen only contains about one fourth of the energy per unit volume as gasoline.

1.5.9. Ultra capacitors

MIT Laboratory for Electromagnetic and Electronic Systems uses nanotubes to improve ultra capacitors. The activated charcoal used in conventional ultra capacitors has many small hollow spaces of various sizes, which create together a large surface to store electric charge. But as charge is quantized into elementary charges, i.e. electrons, and each such elementary charge needs a minimum space, a significant fraction of the electrode surface is not available for storage because the hollow

spaces are not compatible with the charge's requirements. With a nanotube electrode the spaces may be tailored to size—few too large or too small—and consequently the capacity should be increased considerably.

.FINITE ELEMENT MODELING

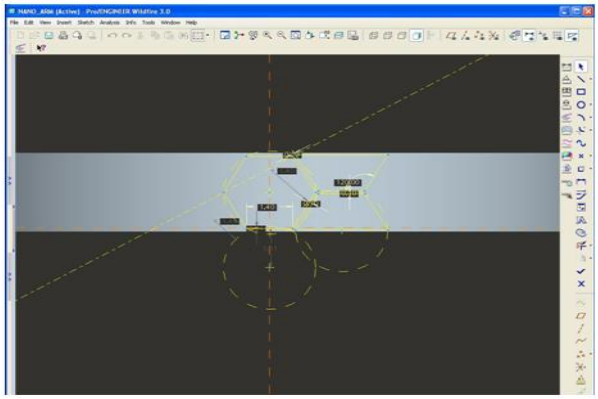

Fig 5.Modeling the base circle for development of arm chair CNT usi

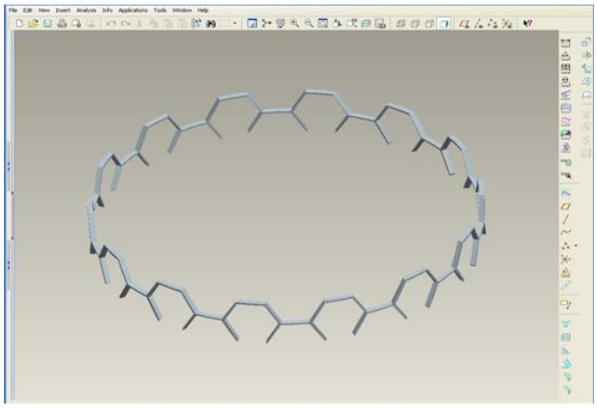

Fig6.Modeling of armchair CNT structure Using pro-e

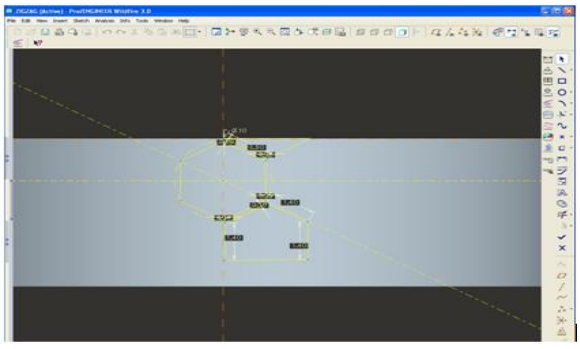

Fig 7.Modeling the base circle for development of zigzag CNT using pro e

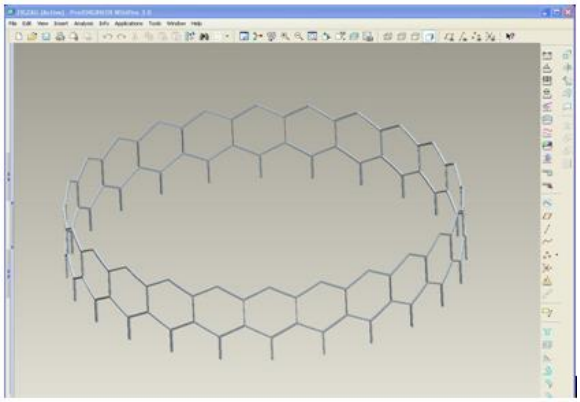

Fig 8.modelling of zigzag CNT structure in pro ENGINEER

Design procedure for meshing of armchair CNT:

- Shell 63 element is used because of the following properties
  1. Shell63 has both bending and membrane capabilities.
  2. Both in-plane and normal loads are permitted.

The element has six degrees of freedom at each node:

- translations in the nodal x, y, and z directions
- Rotations about the nodal x, y, and z-axes.

Stress stiffening and large deflection capabilities are included. A consistent tangent stiffness matrix option is available for use in large deflection (finite rotation) analyses

- The model of armchair carbon nano tube has only one row of the structure of cnt as designed in pro engineer
- using hyper mesh the full structure of cnt is developed.
- finished structure of armchair carbon nano tube is used for further usage.

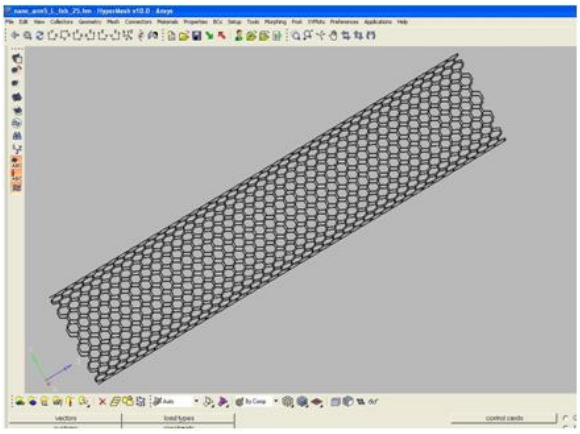

Fig 9 *meshing of armchair CNT*

Design procedure for meshing of zigzag CNT:

- Shell 63 element is used because of the following properties
  - Shell63 has both bending and membrane capabilities.
  - Both in-plane and normal loads are permitted.
  - The element has six degrees of freedom at each node:
- translations in the nodal x, y, and z directions
- Rotations about the nodal x, y, and z-axes.

- Stress stiffening and large deflection capabilities are included.
- A consistent tangent stiffness matrix option is available for use in large deflection (finite rotation) analyses
- The imported model of zigzag carbon nano tube has only one row of the structure of cnt as designed in pro engineer
- using hyper mesh the full structure of cnt is developed
- the finished structure of zigzag carbon nano is used for further usage.

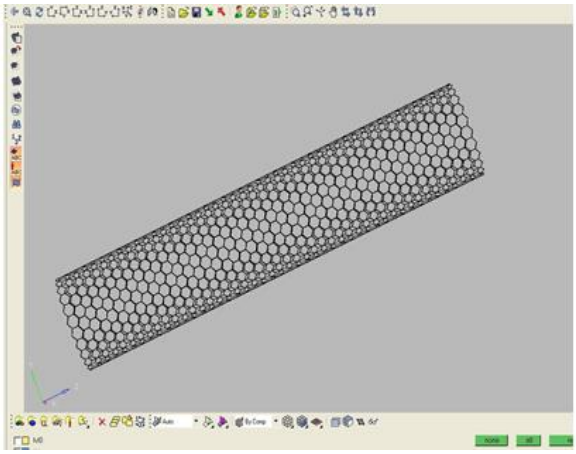

Fig 10 meshing of zigzag CNT

It has been stated that carbon nanotubes are bonded together with covalent bonds which form the hexagonal lattice. These bonds are characterized by bond length and a bond angle. The displacement of individual atoms under the axial force is constrained by the bonds. Therefore, the total deformation of the Nanotube is the result of the interactions between the bonds. The bonds are considered as connecting load carrying elements and the atoms as joints of the connecting elements. The CNTs are simulated as space frame structures. The single walled carbon Nanotube is modeled using the ANSYS 10 software. The wall thickness of the tube is considered to be equal to that of cross sectional diameter of the element. The element chosen is shell which is a combination of spring-slider-damper element. The damping coefficient and the limiting sliding is considered in order to provide an effect of the weak Vander Waals forces in CNTs. In this work the carbon atoms are considered as nodes and the bonds are considered as the elements. The model is meshed and the boundary conditions are applied. The tube is fixed at one end with all degrees of motion arrested at one end and an axial load is applied on the other end.

Design procedure of single wall armchair carbon Nanotube using Ansys:

The procedure can be broadly classified into

Pre processing
Processing (solution)
Post processing

Pre-Processing

Pre processing consists of model generation and discretization into finite elements.

Processing (solution)

After the model is built in pre processing phase, the solution to the analysis is obtained in the processing phase. ts. Boundary conditions are introduced and solution procedures are performed.structural static analysis is used to determine the displacements, stresses, strains and forces that occur in the continuum as a result of applied loads.

Post Processing

Any post processor displays graphically the results in the following modes.

Auto generation-results are presented as charts, tables graphs etc.

The boundary conditions are applied. All degrees of freedom of each node is arrested on one end of the structure while an axial force is applied on each node the other end as shown in fig

Post processing Nodal solution is obtained and the Z-component of displacement is obtained.

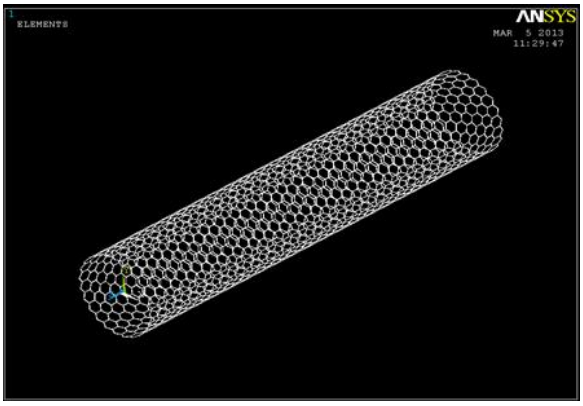

Fig 10 post-processing in ansys

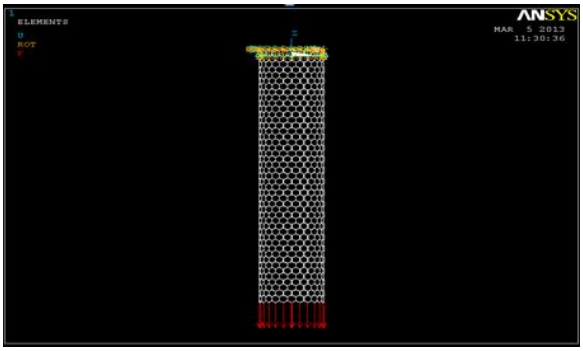

Fig 11 post-processing in ansys

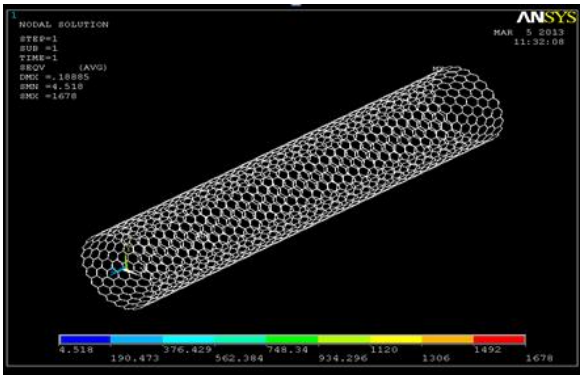

Fig 12 post-processing in ansys

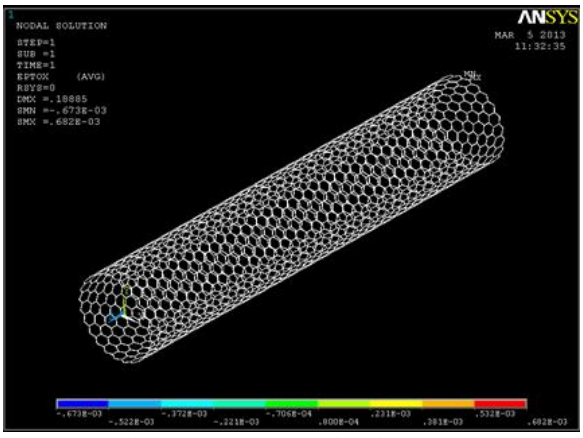

Fig 13 post-processing in ansys

II. Results and Discussions

The potential use of CNTs as reinforcing materials in nano-composites or inpresent advanced composites, originated the need to investigate their mechanical properties.

Two of the properties receiving great attention, because they are appointing the effectiveness of CNTs, are the Young's modulus and tensile strength. Many theoretical and experimental research efforts have been placed on the investigation of Young's modulus of CNTs.

Young's modulus of CNTs either calculated using theoretical methods or measured using experimental techniques show a very wide scatter. The reason for that refers to the physical difficulty of direct experimental measurements, the approximable nature of theoretical methods used and mainly to the dependence of Young's modulus to various geometrical and nano-structural parameters. In the following, the FE model is applied to assess the effect of wall thickness, diameter and chirality on the Young's and shear moduli of SWCNTs.

The Young's modulus of a material is the ratio of normal stress to normal strain as obtained from a uni-axial tension test. Following this definition, the Young's modulus of SWCNTs is been calculated using the following equation

$$Y = \frac{\sigma}{E} = \frac{\frac{F}{A_o}}{\frac{\Delta H}{H_o}}$$

where F is the total applied force,
A0, the cross-sectional area,
H0 the initial length and
DH is the elongation.
A0 is equal to πDt

Where, D is the mean diameter of the tube.

In the case of armchair and zigzag SWCNTs, their initial length H0 is preset since all the sub marginal nodes are situated at the same plane.

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References

[1] Krishnan A, Dujardin E, Ebbesen TW, Yianilos PN, Treacy MMJ (1998). Young's modulus of singlewalled nanotubes. Phys. Rev. B. 58(20):14013–14019.

[2] Li C, Chou TW (2003). A structural mechanics approach for the analysis of carbon nanotubes. J. Solid Struct. 40:2487–2499.

[3] Lourie O, Wanger HD (1998).Evaluation of Young's modulus of carbon nanotubes by micro Raman spectroscopy. J. Mater. 13(9):2418– 2422.

[4] Poncharal P, Wang ZL, Ugarte D, De Heer WA (1999).Electrostatic deflections and electro mechanical resonances of carbon nanotubes. Science 283:1513–1516.

[5] To CWS (2006).Bending and shear moduli of single walled carbon nanotube. Finite Elem. Anal. Des. 42:404–413

[6] Treacy MMJ, Ebbesen TW, Gibson JM (1996). Exceptionally high Young's modulus observed for individual carbon nanotubes. Nature 38(6584):678–680.

[7] Tserpes KI, Papanikos P (2005). Finite element modeling of single walled carbon nanotubes, Composites, Part B. 36:468–477.

[8] Wong EW, Sheehan PE, Lieber CM (1997). Nanobeam mechanics: Elasticity, strength and toughness of nano rods and nanotubes. Science 277:5334.

[9] Yu MF, Files BS, Arepalli S, Ruoff RS (2000a). Tensile Loading of Ropes of Single Wall Carbon Nanotubes and their Mechanical Properties. Phys. Rev. Lett. 84:5552-5555.

[10] Yu MF, Lourie O, Dyer MJ, Moloni K, Kelly TF, Rouff RS (2000b). Strength and breaking mechanism of multi walled carbon nanotube under tensile load. Science 287(5453):637–640.

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