A

Thesis Report

On

TO PROPOSE A METHOD TO IDENTIFY MECHANICAL PROPERTIES OF SINGLE-WALLED CARBON NANOTUBES USING REBO POTENTIAL

Submitted in partial fulfillment of the requirement for the award of degree of

MASTER OF ENGINEERING

In
PRODUCTION & INDUSTRIAL ENGINEERING

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CERTIFICATE

I hereby certify that the work which is being presented in this thesis entitled **"TO PROPOSE A METHOD TO IDENTIFY MECHANICAL PROPERTIES OF SINGLE-WALLED CARBON NANOTUBES USING REBO POTENTIAL"** in partial fulfillment of requirement for the award of Master's Degree in Production & Industrial Engineering submitted in Mechanical Engineering Department, Thapar University, Patiala is an authentic record of the initial work carried out by me under the guidance of Mr. Devender Kumar, Assistant Professor, Mechanical Engineering Department, Thapar University, Patiala.

The matter embodied in this report has not been submitted in part or full to any other university or institute for the award of any degree.

Dated: 16 July 2012

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This is to certify that above declaration made by the student concern is correct to the best of our knowledge & belief.

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ACKNOWLWDGEMENT

I express my sincere gratitude to my guide **Mr. Devender Kumar Assistant Professor Mechanical Engineering Department, Thapar University**, **Patiala,** for their valuable guidance, proper advice and constant encouragement during the course of my work in this seminar.

I express my deep sense of gratitude to **Dr. Ajay Batish, Head of Department, MED** for this inspirational guidance and wholehearted corporation in this area which helps me for successfully carrying the framework of this thesis.

I am also thankful to all my friends who devoted their valuable time and helped me in all possible ways towards successful completion of my thesis work.

I do not find enough words with which I can express my feeling of thanks to the entire faculty and staff of **Mechanical Engineering Department**, **Thapar university**, for their help, inspiration And moral support which went a long way successful completion of my thesis.

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Abstract

The aim of this paper is to propose a Single Walled Carbon Nanotube (SWCNT) approach to evaluate its mechanical properties. With the proposed method, the influence of tube diameter and chirality on the Young's modulus of Single Walled Carbon Nanotubes was investigated. In particular, Zig-Zag carbon nanotubes, with different size, were examined.

According to the Approach 1 the value of Young's Modulus varies from 0.817 to 2.18 TPa, In Approach 2 the values lies in the range from 1.135 to 3.02 TPa and in the Approach 3 the value is in range 1.092 to 2.913 TPa.

The results show that good agreement was achieved with existing experimental results. The presented results demonstrate that the proposed method may also provide a valuable numerical tool for the prediction of the strength behavior of single walled carbon nanotubes.

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Nomenclature

Abbreviations	Description
CNT	Carbon Nanotube
SWNT	Single-Walled Carbon Nanotube
MWNT	Multi-Walled Carbon Nanotube
DWNT	Double Walled Carbon Nanotube
MEMS	Microelectromechanical Systems
NEMS	Nanoelectromechanical Systems
Nm	nano meter
eV	Electron Volt
FET	Field Effect Transducers
GPa	Giga Pascals
TPa	Terra Pascals
a_o	Bond Length
Δr	Change in Bond Length
β	Empirical Constant depends upon a_o
S	Empirical Constant depends upon a_o
Dn	Diameter of Nanotube
m,n	Chiral Vectors
N-nm	Newton Nanometer
MD	Molecular Dynamics

Chapter 1

INTRODUCTION

1.1 Nanotechnology

Nanotechnology is the study of manipulating matter on an atomic and molecular scale. It deals with developing materials, devices, or other structures possessing at least one dimension sized from 1 to 100 nanometers. It is a diverse field ranging from extensions of conventional device physics to completely new approaches based upon molecular self-assembly, from developing new materials with dimensions on the nanoscale to investigating whether we can directly control matter on the atomic scale. Nanotechnology entails the application of fields of science as diverse as surface science, organic chemistry, molecular biology, semiconductor physics, micro fabrication, etc. The emerging field of nanotechnology involves scientists from many different disciplines, including physicists, chemists, engineers, and biologists. There are many interesting Nano devices being developed that have a potential to improve cancer detection, diagnosis, and treatment.[1]

Much of today's nanoscale research is designed to reach a better understanding of how matter behaves on this small scale. The factors that govern larger systems do not necessarily apply at the nanoscale. Because nanomaterials have large surface areas relative to their volumes, Phenomena like friction and sticking are more important than they are in larger systems. Nanotechnology is not new. Nano products are already in the marketplace, such as stain resistant and wrinkle-free textiles. But because it transcends the conventional boundaries between physics, chemistry, biology, mathematics, information technology, and engineering, nanotechnology has the potential to transform the way we live. The disruptive innovations that should arise from nanotechnology over the next decade could be as significant as electricity or the microchip. They could give rise to a whole new set of industries as well as transform current technologies in manufacturing, healthcare, electronics and communications. Importantly, unlike information technology where, for example, consumers might buy a computer, nanotechnology consumers will not buy a 'nanotechnology product' but will buy a product developed or enhanced through nanotechnology.

Examples of exciting applications of nanotechnology include:

- **Nano powders** - The unusual properties of particles less than 100 nm allow a range of new and improved materials with a breadth of applications, such as plastics that behave like ceramics or metals; new catalysts for environmental remediation; improved food shelf-life and packaging; and novel drug delivery devices.

- **Carbon nanotubes** - Graphite can be rolled into a cylinder with a diameter of about 1 nm. These strong but light 'carbon nanotubes' are being developed for a raft of uses, such as sensors, fuel cells, computers and televisions.

- **Nano membrane filtration systems** - These have the potential to address one of the most pressing issues of the 21st Century that is safe, clean, affordable water.

- **Molecular electronic 'cross bar latches'** - Hewlett-Packard believes that silicon computer chips will probably reach a technical dead end in about a decade, to be replaced by tiny Nano devices described as 'cross bar latches'.

- **Quantum dots** - These are small devices that contain a tiny droplet of free electrons essentially artificial atoms. The potential applications are enormous, such as counterfeit-resistant inks, new bio-sensors, quantum electronics, photonics and the possibility of tamper-proof data transmission.

1.1.1 Origin

Nanotechnology is a relatively recent development in scientific research, the development of its central concepts happened over a longer period of time. The emergence of nanotechnology in the 1980s was caused by the convergence of experimental advances such as the invention of the scanning tunneling microscope in 1981 and the discovery of fullerenes in 1985, with the elucidation and popularization of a conceptual framework for the goals of nanotechnology beginning with the 1986 publication of the book Engines of Creation.[2][3] Fullerenes were

discovered in 1985 by Harry Kyoto, Richard Smalley, and Robert Curl, who together won the 1996 Nobel Prize in Chemistry

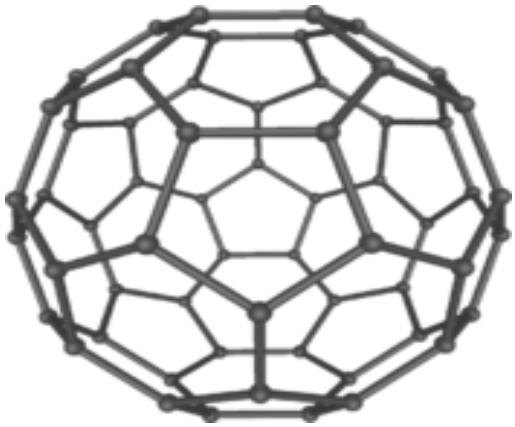

Figure 1: Buckyball

(Buckminsterfullerene C_{60}, also known as the Bucky ball, is a representative member of the carbon structures known as fullerenes. Members of the fullerene family are a major subject of research falling under the nanotechnology umbrella.)

The term "nanotechnology", originally coined by Norio Taniguchi in 1974 but the 1980s the basic idea of this definition was explored in much more depth by Dr. K. Eric Drexler, who promoted the technological significance of Nano-scale phenomena and devices through speeches and the books Engines of Creation: The Coming Era of Nanotechnology (1986) and Nanosystems: Molecular Machinery, Manufacturing, and Computation, and so the term acquired its current sense. Engines of Creation: The Coming Era of Nanotechnology is considered the first book on the topic of nanotechnology. Nanotechnology and nanoscience got started in the early 1980s with two major developments; the birth of cluster science and the invention of the scanning tunneling microscope (STM). This development led to the discovery of fullerenes in 1986 and carbon nanotubes a few years later. In another development, the synthesis and properties of semiconductor nanocrystals was studied, this led to a fast increasing number of metal oxide nanoparticles of quantum dots. The atomic force microscope was invented six years after the STM was invented. In 2000, the United States National Nanotechnology Initiative was founded to coordinate Federal nanotechnology research and development. Today nanotechnology is reshaping technology.

1.1.2 Fundamentals of Nanotechnology

Nanotechnology refers to the projected ability to construct items from the bottom up, using techniques and tools being developed today to make complete, high performance products. One nanometer (nm) is one billionth, or 10^{-9}, of a meter. By convention, nanotechnology is taken as the scale range 1 to 100 nm following the definition used by the National Nanotechnology Initiative in the US. The lower limit is set by the size of atoms (hydrogen has the smallest atoms, which are approximately a quarter of a nm diameter) since nanotechnology must build its devices from atoms and molecules.

To put that scale in another context, the comparative size of a nanometer to a meter is the same as that of a marble to the size of the earth. Or another way of putting it: a nanometer is the amount an average man's beard grows in the time it takes him to raise the razor to his face.

Two main approaches used in nanotechnology are "bottom-up" approach and “top down” approach.

Bottom up Approach – This approach create smaller devices by using larger ones to direct their assembly.

- Technologies that descended from conventional solid-state silicon methods for fabricating microprocessors are now capable of creating features smaller than 100 nm, falling under the definition of nanotechnology.
- Solid-state techniques can also be used to create devices known as nanoelectromechanical systems or NEMS, which are related to microelectromechanical systems or MEMS.
- Focused ion beams can directly remove material, or even deposit material when suitable pre-cursor gasses are applied at the same time. For example, this technique is used routinely to create sub-100 nm sections of material for analysis in Transmission electron microscopy.
- Atomic force microscope tips can be used as a nanoscale "write head" to deposit a resist, which is then followed by an etching process to remove material in a top-down method.

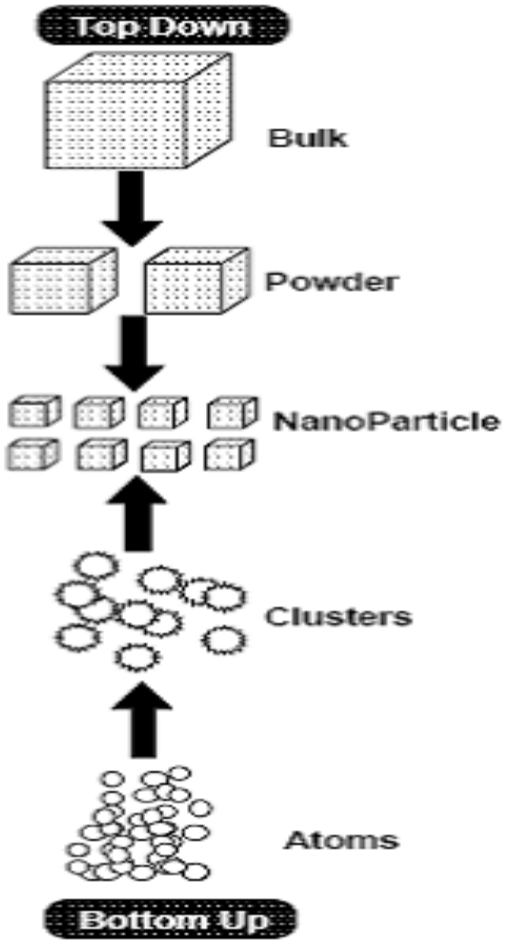

Figure 2: Top Up and Bottom Down Approach

Top down Approach - The "top-down" approach to nanotechnology involves the creation of "Nano-objects" from a parent entity that is larger. This type of fabrication uses lithographic patterning techniques. Unlike bottom-up approach to Nanotechnology that uses the molecular self-assembly chemical process the "top-down" approach uses the traditional workshop or micro fabrication methods with externally-controlled tools.

1.1.3 Key Elements

The technology of realization can be conveniently divided into Fabrication (of materials and devices) and metrology. Both these areas are well covered by other essays in this issue, so here we shall only say a few words about them. Fabrication is divided into ‘top down’ and ‘bottom-

up' techniques. The former constitutes a seamless continuum of processes becoming ever more miniature. There is now considerable overlap between ever more precise cutting and grinding tools (as epitomized by the Cranfield "Tetraform") and the techniques now dominating the integrated circuit industry, in which patterns are transferred (using photolithography or electron beam lithography) onto semiconductors and material is removed by chemical or ion beam etching.

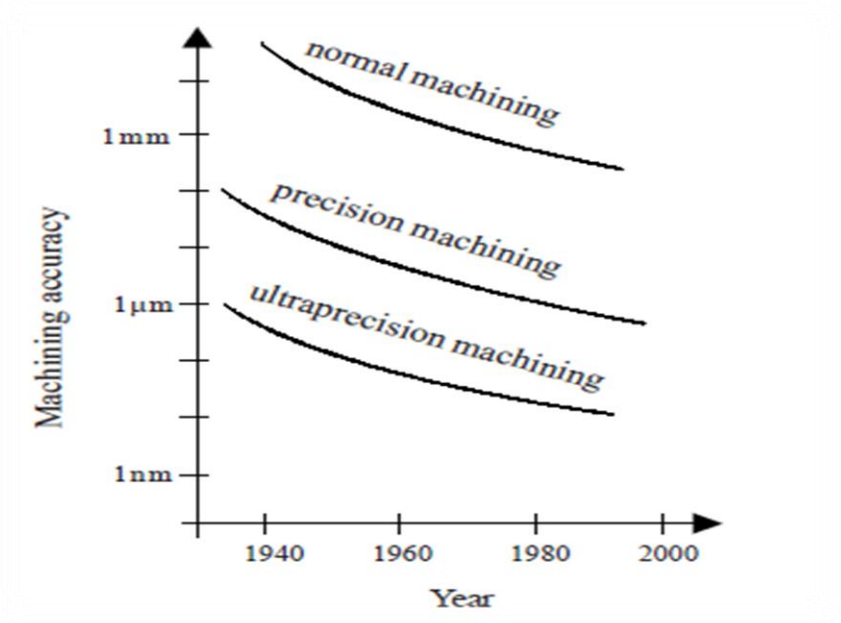

Figure 3: Macining accuracy changes during recent decades

The photolithography family of techniques is hugely expensive, and hence only economical if vast numbers of replicas can be produced. The large capital expense of these fabrication facilities has driven the search for other methods of making ultra-small devices, namely by the process called self-assembly or auto fabrication. This comprises the production of precursors, typically molecules or simply shaped objects that can be produced en masse at low cost, designed such that when they are mixed together in a supporting medium, which might be water or an organic liquid, they connect together in a strictly predefined fashion in order to create complex three dimensional structures. The process is therefore more accurately called self- connecting. An important inspiration for the feasibility of self-connecting fabrication has been the assembly of bacteriophage from precursor structures.

No devices of practical, commercial utility are currently made by this route; however a major difficulty is the current lack of design tools with which manufacturable precursors can be specified for a given final device. Most of the work reported in the field describes structures that were observed to be formed from some interesting precursors. Nevertheless, the much lower capital costs of this fabrication route, and hence the possibility of manufacturing smaller quantities of devices, continues to motivate research work in the field.

Self-connecting processes were studied both experimentally and theoretically long before the appearance of nanotechnology. Although they are considered now to belong to it, as are the 'top down' processes which, since Taniguchi's article, have reached the nanometer scale, the most characteristic Nano technological fabrication process is molecular manufacturing, in which devices are assembled molecule by molecule, or even atom by atom. The assembly would be carried out by purpose-built assemblers, which would themselves be the final products of a chain of machine tool manufacture, in which machines at one level would make the parts for a smaller machine at the subsequent level, as was suggested by R.P. Feynman in his famous 1959 lecture "There's plenty of room at the bottom". Since the assemblers would themselves be very small, they must also be very numerous if they are to be practically useful, hence they should be able to manufacture copies of themselves (lest this self-replicating capability overtaxes their information storage capacity, an alternative would be to reserve the self-replicating ability for the next level up).

1.1.4 What can nanotechnology do?

Nanotechnology is stated to be revolutionary because of three distinct aspects:

- **Indirect** – By this method the progressive miniaturization of existing technologies which opens up new areas of application for those technologies.
- **Direct** – This method refers to the application of novel, Nano engineered artifacts, either to enhance the performance of existing processes and materials
- **Conceptual** - This aspect of nanotechnology, in which all materials and processes are considered from a molecular or even atomic viewpoint, as in living systems, in which complicated molecules (like proteins) are broken down into their constituent amino acids, which are then used for the template synthesis of new proteins

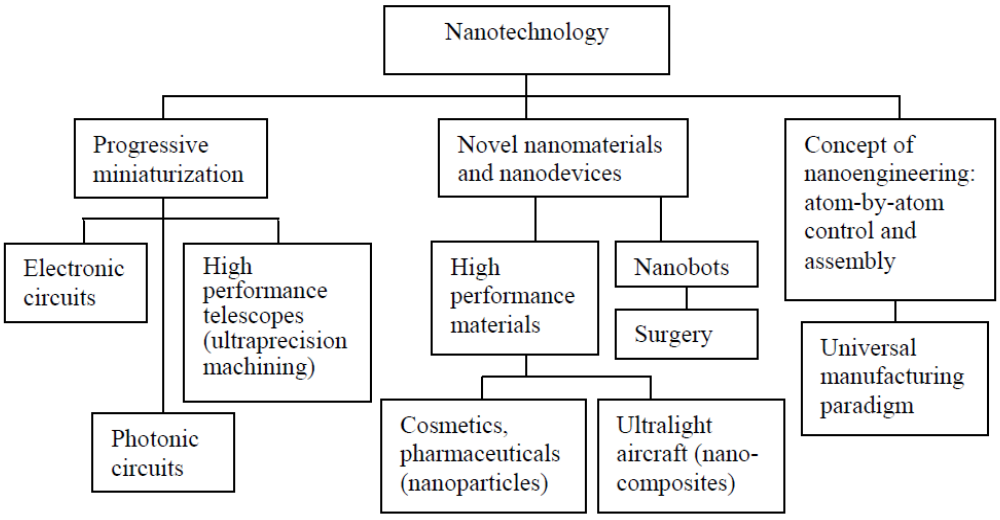

Figure 4: Branches of Nanotechnology

Indirect nanotechnology is enabling technology. Miniaturization can quantitatively enhance performance, and when a quantitative change is big enough, it becomes qualitative. A good example is provided by the history of the cellular telephone. Based on thermionic valves (vacuum tubes), the circuitry for a cellular telephone would take up the volume of a large multistorey building. The cellphone concept—which dates from the 1950s—only became useful once the circuits and their components became small enough to fit into a handset. The minute size of integrated circuit components enables circuits of far greater power and complexity to be realized than would otherwise be practically possible. All the applications of powerful computing, including the World Wide Web, are thus epiphenomena of nanotechnology.

Nanoparticles and Nano sized robots (nanobots) represent direct nanotechnology. There are many advances in this realm whose field of application is such that the Nano component is hidden. A good example is Nano foils made from thousands of alternating nanometer-thick layers of two different metals. A brief electrical pulse applied across the foil initiates mixing of the two metals and the release of a large amount of heat, sufficient for highly localized interfacial bonding of the materials between which the Nano foil is placed. Therefore any assemblage whose components are bonded together using this technique is a manifestation of nanotechnology. The assemblage could be very large, such as an aeroplane.

Finally, by conceptual nanotechnology we mean that nanotechnology represents a novel viewpoint from which to survey the world: one in which structures is scrutinized at the

nanometer scale, and processes are analyzed by considering the movements of each individual atom. This should lead to wholly new ways to understand the world.

1.2 CARBON NANOTUBES

Carbon nanotubes were discovered in 1991 by Sumio Iijima of NEC and are effectively long, thin cylinders of graphite, which you will be familiar with as the material in a pencil or as the basis of some lubricants. Although man often stumbled upon nanomaterials with unique properties but mediaeval stained glass is an example which was apparently done without being aware of the Nano structuring. The properties of steel are now known to be due to structures existing down to the nanometer level, steel was discovered and manufactured largely in ignorance of these structures, and it makes little sense to call steel pioneers such as Bessemer nanotechnologists, any more than it makes sense to call Neanderthal man an early nanotechnologist just because he doubtless produced carbon nanotubes in abundance in his primitive cave fires. Using Nano metrology, these nanotubes are now characterized at unprecedented levels of detail, accompanied by insights from computations.

Carbon nanotubes are one of the most commonly mentioned building blocks of nanotechnology. With one hundred times the tensile strength of steel, thermal conductivity better than all but the purest diamond, and electrical conductivity similar to copper, but with the ability to carry much higher currents, they seem to be a wonder material. However, when we hear of some companies planning to produce hundreds of tons per year, while others seem to have extreme difficulty in producing grams, there is clearly more to this material than meets the eye.

Nanotubes come in many different types as long, short, single-walled, multi-walled, open, closed, with different types of spiral structure, etc. Each type has specific production costs and applications. Some have been produced in large quantities for years while others are only now being produced commercially with decent purity and in quantities greater than a few grams. In this brief white paper we hope to resolve some of the confusion surrounding what may be one of the most significant new materials since plastics. Graphite is made up of layers of carbon atoms arranged in a hexagonal lattice, like chicken wire). Though the chicken wire structure itself is very strong, the layers themselves are not chemically bonded to each other but held together by

weak forces called Van der Waals. It is the sliding across each other of these layers that gives graphite its lubricating qualities.

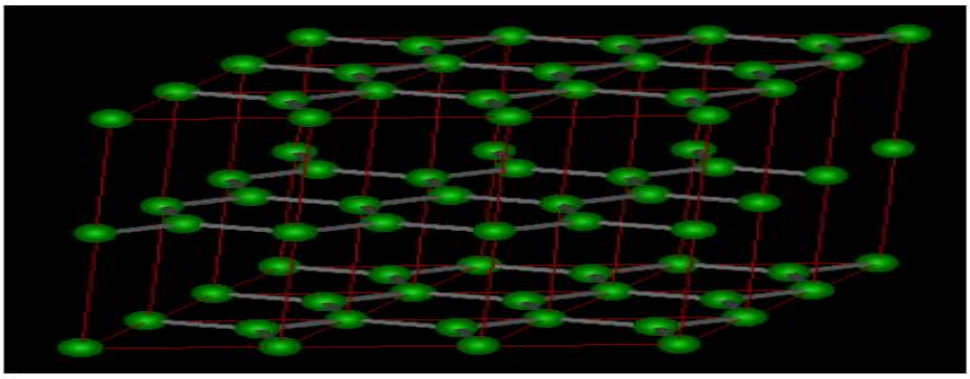

Figure 5: Graphite chicken wire structure

1.2.1 Major classifications of carbon Nanotubes

- Single-walled Carbon Nanotubes (SWNTs), which have a single cylindrical wall
- Multi-walled Carbon Nanotubes (MWNTs), which have cylinders within cylinder

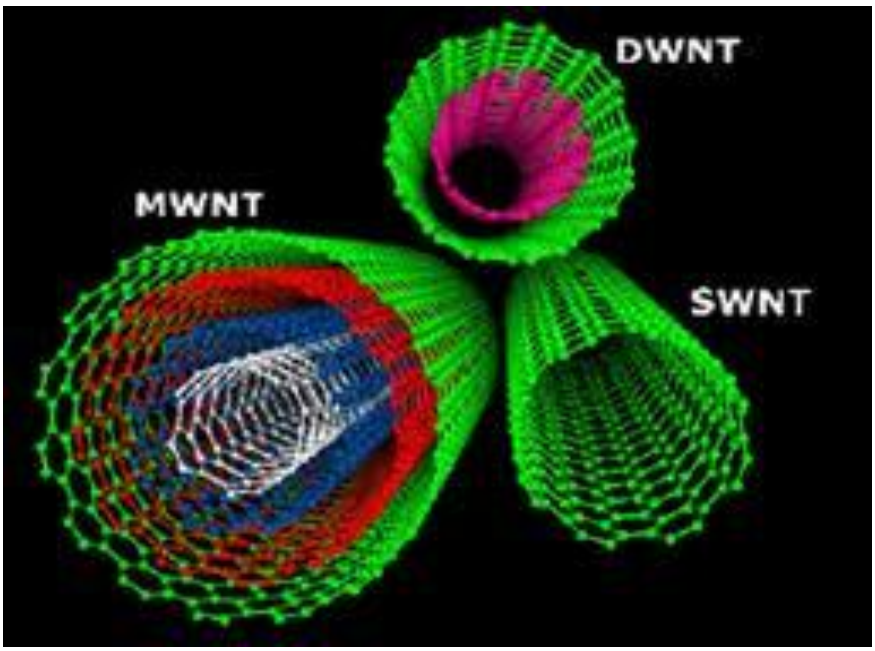

Figure 6: Types of Nanotubes

1.2.1.1 Single-Walled Carbon Nanotubes (SWNTs)

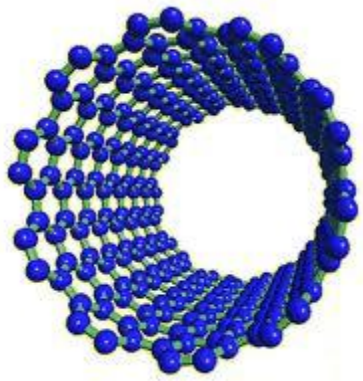

Figure 7: Single walled carbon nanotube

Most single-walled nanotubes (SWNT) 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. The way the graphene sheet is wrapped is represented by a pair of indices (n,m). The integers 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[9].

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

Where a = bond length

SWNTs are an important variety of carbon nanotube because most of their properties change significantly with the (n,m) values, and this dependence is non-monotonic. In particular, their band gap can vary from zero to about 2 eV and their electrical conductivity can show metallic or semiconducting behavior. One useful application of SWNTs is in the development of the first intermolecular field-effect transistors (FET).

1.2.1.2 Multi-Walled Carbon Nanotubes (MWNTs)

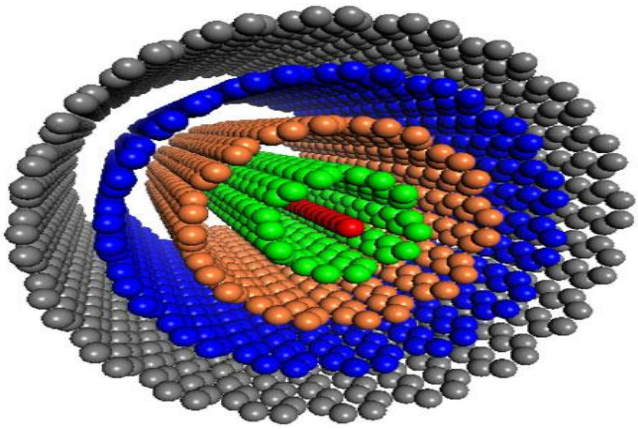

Figure 8: Multi walled carbon nanotubes

Multi-walled nanotubes (MWNT) consist of multiple rolled layers (concentric tubes) of graphite. The interlayer distance in multi-walled nanotubes is close to the distance between graphene layers in graphite, approximately 3.4 Å. Because of statistical probability and restrictions on the relative diameters of the individual tubes, one of the shells, and thus the whole MWNT, is usually a zero-gap metal. Double-walled carbon nanotubes (DWNT) form a special class of nanotubes because their morphology and properties are similar to those of SWNT but their resistance to chemicals is significantly improved. This is especially important when functionalization is required (this means grafting of chemical functions at the surface of the nanotubes) to add new properties to the CNT. In the case of SWNT, covalent functionalization will break some C=C double bonds, leaving "holes" in the structure on the nanotube and, thus, modifying both its mechanical and electrical properties. In the case of DWNT, only the outer wall is modified [10].

1.2.2 Chirality

Imagine a chicken wire fence out of which will be cut a rectangle to roll into a tube, we could cut the rectangle with the sides vertical or at various angles. Additionally, when joining the sides together, we can raise or lower one side. In some cases it will not be possible to make a tube such that the loose ends match and hexagons are formed, but in other cases it will, and these represent the possible permutations of SWNTs.

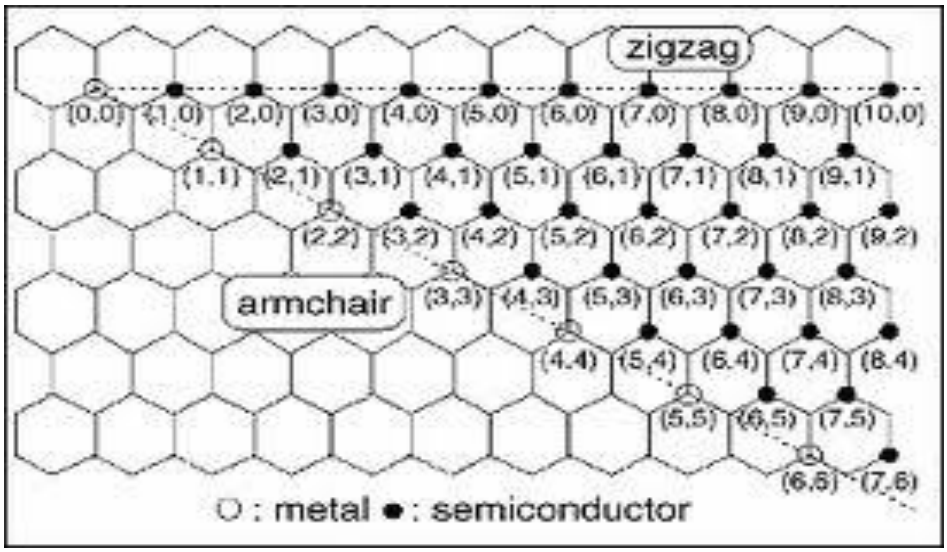

Figure 9: Chirality of nanotubes

The structure of a SWCNT can be conceptualized by wrapping a one-atom-thick layer of graphite (or graphene) into a seamless cylinder. The way the graphene sheet wraps can be represented by a pair of indices (n, m) called the chiral vector. The relationship between n and m defines three categories of CNTs

(i) arm chair (n = m and chiral angle equal to 30°)

(ii) zigzag (n = 0 or m = 0 and chiral angle equal to 0°)

(iii) chiral (other values of n and m and chiral angles lie between 0 and 30°)

1.2.3 Properties

(i) 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. In 2000, a multi-walled carbon nanotube was tested to have a tensile strength of 63 gigapascals (GPa).

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 $kN \cdot m \cdot kg^{-1}$ is the best of known materials, compared to high-carbon steel's 154 $kN \cdot m \cdot kg^{-1}$. Under excessive tensile strain, the tubes will undergo plastic deformation,

which means the deformation is permanent. This deformation begins at strains of approximately 5% and can increase the maximum strain the tubes undergo before fracture by releasing strain energy. 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[11][12].

Table 1: Comparison of Young's modulus and tensile strength of carbon nanotubes with other materials

Material	Young's Modulus (GPa)	Tensile Strength (GPa)	Density (g/cu.cm.)
Single wall nanotube	1054	150	1.4
Multi wall nanotube	1200	150	2.6
Diamond	600	130	3.5
Kevlar	186	3.6	7.8
Steel	208	1.0	7.8
Wood	16	0.008	0.6

(ii) Hardness

Standard single-walled carbon nanotubes can withstand a pressure up to 24GPa without deformation. They then undergo a transformation to super hard phase nanotubes. Maximum pressures measured using current experimental techniques are around 55GPa. However, these new super hard phase nanotubes collapse at an even higher, albeit 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)[13].

(iii) Kinetic

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.[14]

(iv) Electrical

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[15][16].

(v) Optical

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. [8]

(vi) Thermal

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 $W \cdot m^{-1} \cdot K^{-1}$; compare this to copper, a metal well known for its good thermal conductivity, which transmits 385 $W \cdot m^{-1} \cdot K^{-1}$. A SWNT has a room-temperature thermal conductivity across its axis (in the radial direction) of about 1.52 $W \cdot m^{-1} \cdot K^{-1}$, 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.[17]

(vii) Wave Absorption

The most recently researched properties of multi-walled carbon nanotubes (MWNTs) are their wave absorption characteristics, specifically microwave absorption. There has been some research on filling MWNTs with metals, such as Fe, Ni, Co, etc., to increase the absorption effectiveness of MWNTs in the microwave regime. This research has shown improvements in both maximum absorption and bandwidth of adequate absorption.

1.2.4 Defects

The existence of a crystallographic defect affects the material properties. Defects can occur in the form of atomic vacancies. High levels of such defects can lower the tensile strength by up to 85%. An important example is the Stone Wales defect, which creates a pentagon and heptagon pair by rearrangement of the bonds. Because of the very small structure of CNTs, the tensile strength of the tube is dependent on its weakest segment in a similar manner to a chain, where the strength of the weakest link becomes the maximum strength of the chain.

Crystallographic defects also affect the tube's electrical properties. A common result is lowered conductivity through the defective region of the tube. These strongly affect the tube's thermal properties. Such defects lead to phonon scattering, which in turn increases the relaxation rate of the phonons. This reduces the mean free path and reduces the thermal conductivity of nanotube structures. Larger-scale defects such as Stone Wales defects cause phonon scattering over a wide range of frequencies, leading to a greater reduction in thermal conductivity[18][19].

1.2.5 Potential Applications of CNT's

(i) Structural

- Textiles - CNT can make waterproof and/or tear-resistant fabrics.
- Body armor - MIT is working on combat jackets that use CNT fibers to stop bullets and to monitor the condition of the wearer. Cambridge University developed the fibers and licensed a company to make them.

- Concrete - CNT in concrete increase its tensile strength, and halt crack propagation.
- Polyethylene - Adding CNT to polyethylene can increase the polymer's elastic modulus by 30%.
- Sports equipment - Stronger and lighter tennis rackets, bicycle parts, golf balls, golf clubs, and baseball bats.
- Space elevator - CNT are under investigation as possible components of the tether up which a space elevator can climb. This requires tensile strengths of more than about 70 GPa.
- Synthetic muscles - Due to their high contraction/extension ratio given an electric current, CNTs are ideal for synthetic muscle.
- High tensile strength fibers - Fibers produced with polyvinyl alcohol required 600 J/g to break. In comparison, the bullet-resistant fiber Kevlar fails at 27–33 J/g.
- Bridges - CNT may be able to replace steel in suspension and other bridges.
- Flywheels - The high strength/weight ratio enables very high rotational speeds.
- Carbon nanotube springs - Single-walled carbon nanotubes aligned in parallel can be elastically stretched for an energy density 10 times greater than that of current lithium-ion batteries, with the additional advantages of long cycling durability, temperature insensitivity, no spontaneous discharge, and arbitrary discharge rate.
- Fire protection - Thin layers of Bucky paper can significantly improve fire resistance due to the efficient reflection of heat by the dense, compact layer of CNT or carbon fibers[20][21][22].

(ii) Electromagnetic

- Artificial muscles - CNT's have sufficient contractility to make them candidates to replace muscle tissue.
- Bucky paper - Thin nanotube sheets are 250 times stronger than steel and 10 times lighter and could be used as a heat sink for chipboards, a backlight for LCD screens or as a faraday cage to protect electrical devices/aeroplanes.
- Chemical nanowires - CNTs can be used to produce nanowires of other elements/molecules, such as gold or zinc oxide. These nanowires in turn can be used to cast nanotubes of other chemicals, such as gallium nitride.

- Conductive films - Nanotube films show promise for use in displays for computers, cell phones, Personal digital assistants, and automated teller machines.
- Electric motor brushes - Conductive CNTs are used in brushes for commercial electric motors. They replace traditional carbon black.
- Light bulb filament - Alternative to tungsten filaments in incandescent lamps.
- Magnets - Multi-walled nanotubes coated with magnetite can generate strong magnetic fields.
- Optical ignition - A layer of 29% iron enriched single-walled nanotubes (SWNT) is placed on top of a layer of explosive material such as PETN, and can be ignited with a regular camera flash.
- Superconductor - Nanotubes have been shown to be superconducting at low temperatures.
- Ultra capacitors - MIT is researching the use of nanotubes bound to the charge plates of capacitors in order to dramatically increase the surface area and therefore energy storage ability.
- Displays - CNTs can be used as extremely fine electron guns, which could be used as miniature cathode ray tubes in thin high-brightness, low-energy, and low-weight displays.

(iii) Chemical

- Desalination - Water molecules can be separated from salt by forcing them through networks of carbon nanotubes, which require far lower pressures than conventional reverse osmosis methods.
- Air pollution filter - CNT membranes can filter carbon dioxide from power plant emissions.
- Biotech container - CNT can be filled with biological molecules, aiding biotechnology.
- Hydrogen storage - CNT have the potential to store between 4.2 and 65% hydrogen by weight. If they can be mass produced economically, 13.2 litres (2.9 imp gal; 3.5 US gal) of CNT could contain the same amount of energy as a 50 liters (11 imp gal; 13 US gal) gasoline tank.

(iv) Mechanical

- Oscillator - Oscillators based on CNT have achieved higher speeds than other technologies (> 50 GHz).
- Nanotube membrane - Liquid flows up to five orders of magnitude faster than predicted by classical fluid dynamics.
- Slick surface - Some CNT-based fabrics have shown lower friction than Teflon.
- Waterproof - Some CNT-fabrics are waterproof.
- Infrared detector - The reflectivity of the Bucky paper produced with "super-growth" chemical vapor deposition method is 0.03 or less, potentially enabling performance gains for pyro electric infrared detector.
- Thermal radiation - For thermal emission in space such as space satellites.
- Stealth - Absorbance is high in wide ranges from FUV to FIR.

(v) Electrical Circuits

A nanotube formed by joining two nanotubes of different diameters end to end can act as a diode, suggesting the possibility of constructing computer circuits entirely of nanotubes. Because of their good thermal transmission properties, CNT can potentially dissipate heat from computer chips. The longest electricity conducting circuit is a fraction of an inch long.

(vi) Medicine

Carbon nanotubes (CNTs) are very prevalent in today's world of medical research and are being highly researched in the fields of efficient drug delivery and bio sensing methods for disease treatment and health monitoring. Carbon nanotube technology has shown to have the potential to alter drug delivery and bio sensing methods for the better, and thus, carbon nanotubes have recently garnered interest in the field of medicine.

The use of CNTs in drug delivery and bio sensing technology has the potential to revolutionize medicine. Functionalization of SWNTs has proven to enhance solubility and allow for efficient tumor targeting/drug delivery. It prevents SWNTs from being cytotoxic and altering the function of immune cells. Cancer, a group of diseases in which cells grow and divide abnormally, is one

of the primary diseases being looked at with regards to how it responds to CNT drug delivery. The high electrochemically accessible surface area, high electrical conductivity and useful structural properties have demonstrated the potential use of single-walled nanotubes (SWNTs) and multi-walled nanotubes (MWNTs) in highly sensitive noninvasive glucose detectors.

(vii) 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.

- **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. 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. As a threshold for economical storage, the Department of Energy has set 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).
- **Lithium Intercalation -** The basic principle of rechargeable lithium batteries is electrochemical intercalation and deintercalation of lithium in both electrodes. An ideal battery has a high-energy capacity, fast charging time and a long cycle time. The capacity is determined by the lithium saturation concentration of the electrode materials. For Li, this is the highest in nanotubes if all the interstitial sites (inter-shell van der Waals spaces, inter-tube channels and inner cores) are accessible for Li intercalation. SWNTs have shown to possess both highly reversible and irreversible capacities. Because of the large observed voltage hysteresis, Li-intercalation in nanotubes is still

unsuitable for battery application. This feature can potentially be reduced or eliminated by processing, i.e. cutting, the nanotubes to short segments.

- **Electrochemical Supercapacitors** - Supercapacitors have a high capacitance and potentially applicable in electronic devices. They are comprised two electrodes separated by an insulating material that is ionically conducting in electrochemical devices. The capacity of an electrochemical supercap inversely depends on the separation between the charge on the electrode and the counter charge in the electrolyte. Because this separation is about a nanometer for nanotubes in electrodes, very large capacities result from the high nanotube surface area accessible to the electrolyte. In this way, a large amount of charge injection occurs if only a small voltage is applied. This charge injection is used for energy storage in nanotube supercapacitors.

Table 2: Types of hydrogen stores

Storage Medium	Temperature respective pressure	Mass respective volume	Storage Capacity	Advantages & Disadvantages
Liquid Hydrogen	-270ºC	140 kg, 86 l	7,5 weight%	• + Small volume • - Very expensive insulation • - Energy loss by gas liquefaction • - Gas leakage during storage
Gaseous Hydrogen	700 bar	125 kg, 260 l	6 weight%	• + Low technical effort • - High vol. req. for cylindrical high pr. Tanks • - Safety risks for high pr.

Nanoscale Metal Hydrides (e.g. MgH_2)	>300ºC, 800 bar	175 kg, 73 l	4-7 weight%	• + Low volume req. • - High weight • - Req. very high temp.
Nanoporous metal organic materials (MOF_s)	<-210ºC, >50 bar	86 kg, 160 l	7,5 weight%	• + Low weight • - Low temp. • - High vol. req.

1.3 REBO Potential

It stands for Reactive Empirical Bond Order Potential. It is an analytic potential energy function for solid carbon and hydrocarbon molecules based on a reactive empirical bond order (REBO) formalism is presented. This formalism allows for covalent bond breaking and creation with associated changes in atomic hybridization within a classical potential, producing a powerful method for modeling complex chemistry in large many-body systems. The potential energy functions are simplified mathematical expressions that attempt to model interatomic forces arising from the interaction of electrons and nuclei.

For being be effective, an analytic potential energy function must possess the following critical properties:

1. *Flexibility*: A potential energy function must be sufficiently flexible so that it accommodates as wide a range as possible of fitting data.

2. *Accuracy*: A potential should be able to accurately reproduce an appropriate fitting data base.

3. *Transferability*: A potential function should be able to describe at least qualitatively, if not with quantitative accuracy, structures not included in a fitting data base.

4. *Computational efficiency*: Evaluation of the function should be relatively efficient depending on quantities such as system sizes and timescales of interest, as well as available computing resources.

The analytic bond order potential was introduced by Abell. The general expression for the Rebo potential is as following:

$$\mathbf{V} = \sum \boldsymbol{V_R} - \boldsymbol{\beta_{ij}} \sum \boldsymbol{V_A}$$

$$\boldsymbol{V_R} = \mathbf{(De/S-1)^* \exp[-\sqrt{(2S)}^* \beta^* \Delta r]}$$

$$\boldsymbol{V_A} = \mathbf{(DeS/S-1)^* \exp[-\sqrt{(2/S)}^* \beta^* \Delta r]}$$

$V_R \; and \; V_A$ are pair additive repulsive and attractive interaction, respectively. B_{ij} represents a many-body coupling between the bond from atom *i* to atom *j* and local environment of atom *i*, it can be considered a normalized bond order because the Pauling relationship between bond order and bond length is realized. S and β are the empirical constants and De is the potential well depth.

$$\boldsymbol{B_{ij}} \; \boldsymbol{\alpha} \; \boldsymbol{Z^{-\delta}}$$

CHAPTER 2

2.1 Literature Review

The literature survey has been conducted to survey on the following area:

Aleksander Muc (2009) has done work on methods of design and identification of mechanical properties carbon nanotubes. According to him atomic arrangement and configuration of carbon nanotubes (CNTs) imposes the necessity of the use of transversely isotropic or especially orthotropic material models in the description of their effective material properties instead of isotropic one. Therefore, in the present paper an identification technique based on the analysis of natural vibrations is introduced. Theoretical values of natural vibrations are derived with the use of theoretical relations valid for thin orthotropic cylindrical shells. They are compared with numerical ones calculated utilizing a three-dimensional finite element (FE) model for armchair and zigzag single-walled carbon nanotubes (SWCNTs). The numerical model development is consistent with molecular mechanics formulations and it is based on the assumption that carbon nanotubes, when subjected to free vibrations, behave like space-frame structures. In order to compare the numerical and theoretical values of eigen frequencies two forms of the interatomic potentials are considered: the modified Morse potential and REBO potential. In order to avoid local modes of deformations the axisymmetric modes are investigated only. A detailed study of results demonstrates that CNTs should be considered as orthotropic structures[1].

P. Zhang et. al. (2002) says a nanoscale continuum theory is established to directly incorporate interatomic potentials into a continuum analysis without any parameter fitting. The theory links interatomic potentials and atomic structure of a material to a constitutive model on the continuum level. The theory is applied to study the linear elastic modulus of a single-wall carbon nanotube. The Young's modulus predicted by this nanoscale continuum theory agrees well with prior experimental results and atomistic studies. A nanoscale continuum theory has been established to directly incorporate the interatomic potential into the continuum analysis of the solids. Once the interatomic potential and the atomic structure of the material are known, a systematic approach, which does not involve any parameter fitting, has been proposed to link the

constitutive model on the continuum level to the interatomic potential of the material with the Centro symmetric atomic structure. [2].

Dong Qian et. al. (2002) reviewed the theoretical predictions and discuss the experimental techniques that are most often used for the challenging tasks of visualizing and manipulating these tiny structures. We also outline the computational approaches that have been taken, including ab initio quantum mechanical simulations, classical molecular dynamics, and continuum models.

The development of multiscale and multiphysics models and simulation tools naturally arises as a result of the link between basic scientific research and engineering application; while this issue is still under intensive study, we present here some of the approaches to this topic. Our concentration throughout is on the exploration of mechanical properties such as Young's modulus, bending stiffness, buckling criteria, and tensile and compressive strengths.

Finally, they discussed several examples of exciting applications that take advantage of these properties, including nanoropes, filled nanotubes, nanoelectromechanical systems, nanosensors, and nanotube-reinforced polymers [3].

Jean-Paul Salvetat (1999) used an atomic force microscope and a special substrate, the elastic and shear moduli of individual single-walled nanotube (SWNT) ropes were measured to be of the order of 1 TPa and 1 GPa, respectively. In contrast to multiwalled nanotubes, unexpectedly low intertube shear stiffness dominated the flexural behavior of the SWNT ropes. This suggested that intertube cohesion should be improved for applications of SWNT ropes in high-performance composite materials. From small diameter and long ropes was deduced an elastic modulus of about 1 TPa. The AFM measurements thus confirmed that carbon nanoropes are high-modulus fibers but with an unexpectedly low shear modulus (G ø 1 GPa). This should be taken into account in the design of nanorope-based composite materials. It would be particularly interesting to cross-link the nanotubes in a rope, for example, by irradiation or chemical methods, to increase the rigidity of a rope. [4].

K.S. Challagulla (2008) developed a comprehensive micromechanical model for the analysis of periodic thin composite shells with an embedded grid of generally orthotropic reinforcements.

The use of composite and smart composite structures in existing and new engineering applications will be significantly facilitated if the effective properties and coefficients such as elastic, piezoelectric, thermal expansion etc. can be predicted at the design stage. To achieve this goal, mathematical models characterizing the behavior of the said structures is developed. The use of generally orthotropic constituents renders the analysis more complicated than with simply isotropic reinforcements, but significantly enhances the applicability of the model. The model is derived on the basis of asymptotic homogenization and allows the determination of the effective elastic. The developed model is illustrated by means of several examples including cylindrical reinforced shells, single-walled carbon nanotubes, multi-layered shells, and rectangular and triangular network reinforced thin composite plates. In the case of carbon nanotubes, closed-form expressions for the longitudinal (ENT) and shear (GNT) moduli are obtained. In the case of multi-layered shells and grid reinforced plates, it is shown that the model can be used to tailor the effective elastic coefficients of the structures to conform to any application by changing some material or geometric parameters of interest such as the type, number, dimensions and angular orientation of the reinforcements. [5].

T. Belytschko et. al. (2002) The molecular mechanics and molecular dynamics studies of the failure of nanotubes have been reported here. The equilibrium configuration of the model system is sought by minimizing the energy, which consists of the sum of the interatomic potentials minus any work by external forces. Such methods imply a temperature of 0 K and cannot account for the effects of temperature. In molecular dynamics methods, the momentum equations are integrated in time for the system of atoms with interatomic forces given by the interatomic potential. The fracture of carbon nanotubes is studied by atomistic simulations. The fracture behavior is found to be almost independent of the separation energy and to depend primarily on the inflection point in the interatomic potential. The range of fracture strains compares well with experimental results, but the predicted range of fracture stresses is markedly higher than observed. Various plausible small-scale defects do not suffice to bring the failure stresses into agreement with available experimental results. As in the experiments, the fracture of carbon nanotubes is predicted to be brittle. The results show moderate dependence of fracture strength on chirality [6].

Eric W. Wong et. al. (1997) The Young's modulus, strength, and toughness of nanostructures are important to propose applications ranging from Nano composites to probe microscopy, yet there is little direct knowledge of these key mechanical properties. Atomic force microscopy was used to determine the mechanical properties of individual, structurally isolated silicon carbide (SiC) Nano rods (NRs) and multiwall carbon nanotubes (MWNTs) that were pinned at one end to molybdenum disulfide surfaces. The bending force was measured versus displacement along the unpinned lengths. The MWNTs were about two times as stiff as the SiC NRs. Continued bending of the SiC NRs ultimately led to fracture, whereas the MWNTs exhibited an interesting elastic buckling process. The strengths of the SiC NRs were substantially greater than those found previously for larger SiC structures, and they approach theoretical values. Because of buckling, the ultimate strengths of the stiffer MWNTs were less than those of the SiC NRs, although the MWNTs represent a uniquely tough, energy-absorbing material [7].

Uttandaraman Sundaraj et. al. (2004) Carbon nanotubes are promising new materials for blending with polymers with potential to obtain low-weight nanocomposites of extraordinary mechanical, electrical, thermal and multifunctional properties. The size scale, aspect ratio and properties of nanotubes provide advantages in a variety of applications, including electrostatically dissipative materials; advanced materials with combined stiffness, strength and impact for aerospace or sporting goods; composite mirrors; automotive parts that require electrostatic painting and automotive components with enhanced mechanical properties. The various processing methods for producing these nanocomposites are discussed, in particular melt mixing, solution processing and in-situ polymerization [8].

Mahmoud Nadim et. al. (2010) developed a finite element model to study the mechanical behavior of nano-structured materials. The model serves as a link between computational chemistry and solid mechanics by substituting discrete molecular structures with an equivalent-continuum model. The model reported here is a continuation of a previous model, which was developed by the authors and was applied to determine the effective stiffness of a graphene sheet. The present model is developed by bending the previously developed graphene sheet

model around its vertical edge to form a single wall carbon nanotube, which, then, has been characterized to find its mechanical properties [9].

Pulickel M. Ajayan et. al. (2001) described some of the important materials science applications of carbon nanotubes. They discuss the electronic and electrochemical applications of nanotubes, nanotubes as mechanical reinforcements in high performance composites, nanotube-based field emitters, and their use as Nano probes in metrology and biological and chemical investigations, and as templates for the creation of other nanostructures. Electronic properties and device applications of nanotubes are treated elsewhere in the book. The challenges that ensue in realizing some of these applications are also discussed from the point of view of manufacturing, processing, and cost considerations [10].

Chunyu Li. Et. al. (2005) The stress distributions in carbon nanotube clamps such as those formed by the electron beam induced deposition (EBID) technique are analyzed and the contributing factors, including nanotube position, stiffness of clamp material, and thickness of the clamping pad between the AFM tip and the nanotube are examined for the case of tensile loading of the nanotube. The nanotube is modeled at the atomistic scale by the molecular structural mechanics approach and is assumed to be defect free. The clamp material is analyzed by the continuum finite element method. The nanotube and the clamp are assumed to be bonded perfectly to each other. This bonding condition sets the upper limit of clamping capacity. The simulation results indicate that the location and intensity of stress concentration are sensitive to the nanotube orientation. Misaligned nanotubes are likely to break near the edge of the clamp. The clamp material with a lower stiffness (for the stiffness range studied) and a thicker clamping pad between the nanotube and the AFM tip reduce the magnitude of stress concentrations in the clamp [11]

Marko Canadija et. al. (2009) gave a theory of multi-walled carbon nanotubes and a suitable way for modeling them using the finite element method. A brief reference to FE modeling of a single walled carbon nanotube (SWNT) is given as an introduction to modeling of multi-walled carbon nanotubes, consisting of several layers of SWNT. Also, a theory of the connection interface between nanotube layers and its influence on the loading is given. A SWNT finite

element model is used to model a multi-walled carbon nanotube (MWNT). A brief theory concerning MWNT is given, as well as a theory of modeling a connecting interface between layers, as a result of van der Waals interactions. Different loading conditions are used as examples of multi-walled carbon nanotubes under specific loads. Results are compared with those given by other authors [12].

Mehrdad Arjmand Et. Al.(2010) developed an analytical molecular structural mechanics model for the prediction of Young's modulus of zigzag single walled carbon nanotubes with single vacancies by combining continuum mechanics with modified Morse potential function under tensile loading. The defects like vacancies cause a remarkable change in the Young's modulus, especially when they are numerous. The effects of defect concentration in the axial direction (length of defective section(s) /total length of the tube) and defect concentration in the transverse direction (number of vacancies in circumference) on Young's modulus have been studied. By increasing diameter the effect of defects is decreased and modulus of defective CNTs approaches that of an intact CNT. Combining continuum mechanics with atomistic potential functions has made this research unique. The Young's modulus of an intact CNT is in good agreement with most recent research and is an indication of the value of the theory. [13]

K. Udhaya Kumar (2011) presented the computational studies about the mechanical and transport properties of armchair (4, 4) and zigzag (4, 0) single walled carbon nanotubes. Carbon nanotubes are so small that changes in structure can affect the Young's modulus. For an armchair and zigzag single walled carbon nanotube Young's Modulus are calculated using an atomistic approach and density functional theory (DFT). Atomic forces and total energies for strained carbon nanotube segments are computed using Atomistix's Virtual Nano Lab (VNL) and Toolkit (ATK) software. For a maximum strain of one percent, elastic moduli are calculated using both force-strain and energy-strain data. Young's modulus is in the range 1.8 to 4.17 TPa depending on the cross-sectional area taken for the carbon nanotube.[14]

Michael Griebel et. al. (2005) examined the elastic properties of boron-nitride nanotubes, which are embedded in amorphous silicon-boron-nitride ceramics. They employed molecular dynamics simulations using the Parrinello-Rahman approach. To this end, all systems are modeled with a

reactive many-body bond order potential due to Tersoff, which is able to describe covalent bonding accurately external stress and derive stress-strain curves for various tensile and compressive load cases at given temperature and pressure. In addition to Young moduli and Poisson ratios, radial distribution functions, average coordination numbers, ring statistics and self-diffusion coefficients were compared to characterize the short-range, medium-range and long-range order of Si3BN5, Si3B2N6 and Si3B3N7 matrices, respectively. Here, our results show that Si3B3N7 exhibits the highest Young modulus and the largest elastic range.

The properties of a ceramics composite material made from Si3B3N7 matrix and BN nanotubes were studies and calculated stress-strain curves for the composite to predict the rates of reinforcement of the matrix due to the BN nanotubes. The influence of the nanotube/matrix-ratio on the elastic modulus of the composite is examined. Finally, the Young moduli derived from numerical simulations is compared to predictions given by both, a simple macroscopic rule-of-mixtures, which depends on the volume fraction only, and an extended rule-of-mixtures, which also takes the geometry of the BN nanotube into account. The numerical results obtained show that the extended rule-of-mixtures predicts the Young modulus of the composite with a relative error of 5% or less. The simulation results show that BN nanotubes can be used to reinforce Si-B-N ceramics. [15]

J. Cumings et. al. (2002) demonstrated that boron nitride (BN) nanotubes can be filled "peapod" fashion with C60 molecules. Filling small-diameter BN nanotubes results in a linear chain of C60 molecules in the interior, while filling large diameter BN nanotubes leads to nanorods of crystalline C60 in the interior. Electron beam damage can be used to fuse the encapsulated C60 molecules into carbon nanotubes, leading to carbon nanotubes encased within insulating BN nanotubes. BN nanotubes can also be synthesized with mobile magnetic nanocrystals within their core. [16]

W. Mickelson et. al. (2002) Crystal structure is key in determining the mechanical, electronic, thermal, and magnetic properties of materials. Silicon, for example, is a modest bandgap semiconductor in its common diamond structure, but in its high pressure simple hexagonal structure it is a metal and a superconductor. C60 nanowire were created by packing C60 molecules into the interior of insulating boron nitride nanotubes (BNNTs).For small-diameter

BNNTs, the wire consists of a linear chain of C60 molecules. With increasing BNNT inner diameter, unusual C60 stacking configurations are obtained (including helical, hollow core, and incommensurate) that are unknown for bulk or thin-film forms of C60. C60 in BNNTs thus presents a model system for studying the properties of dimensionally constrained "silo" crystal structures. For the linear-chain case, we have fused the C60 molecules to form a single walled carbon nanotube inside the insulating BNNT. [17]

Chung-Jung Wu et. al. (2011) The notable material properties of carbon nanotubes (CNTs) with ballistic electrical transport, ultrahigh Young's modulus and thermal conductivity made them very attractive for microelectronic interconnections, thermal management and nanoscale device applications. This paper focuses on the analysis of mechanical properties of single-walled carbon nanotubes (SWCNTs). The atomistic continuum mechanics (ACM) was applied to investigate the mechanical properties of SWCNTs. By establishing a linkage between structural mechanics and molecular mechanics, not only the Young's moduli could be obtained but also the modal analysis could be achieved. [18]

K T Kashyap et. al. (2007) Carbon nanotubes are the ultimate carbon fibers because of their high Young's modulus of ≈ 1 TPa which is very useful for load transfer in nanocomposites. In the paper CNT/Al nanocomposites were fabricated by the powder metallurgy technique and after extrusion of the nanocomposites bright field transmission electron microscopic (TEM) studies were carried out. From the TEM images so obtained, a novel method of ascertaining the Young's modulus of multi-walled carbon nanotubes is found out which turns out to be 0·9 TPa which is consistent with the experimental results. [19]

Douglas Vodnik et. al. (2007) A new numerical method for calculating the Young's modulus of carbon nanotubes which avoids ambiguities that have plagued other attempts is validated. Molecular dynamics simulations that utilize the Tersoff Potential are used to model various single-walled carbon nanotubes under different strains to achieve this validation. Data is taken from an armchair, zigzag, and chiral carbon nanotube. The calculated Young's moduli are all around Y = 1 TPa, in agreement with existing experimental data. [20]

Kaveh PourAkbar Saffar et. al. (2008) The presence of chemical bonding between functionalized carbon nanotubes and matrix in carbon nanotube reinforced composites is modeled by elastic beam elements representing covalent bonding characteristics. Neglecting other reinforcing mechanisms in the composite such as relatively weak interatomic Van der Waals forces, this model shows close results to the Rule of Mixtures model's prediction for effective Young's modulus of a Representative Volume Element of composite for small volume fractions (~1%) and high aspect ratios (L/D>200) of CNTs. Current model is valid for elastic linear assumption for cross-links and thus, is applicable to the atomic bond force linearly related to atoms separation distance but not for large bond strains in which the atomic forces show nonlinear behavior with respect to atoms separation distance. [21]

Andras Kis et. al. (2008) Superior mechanical properties of CNTs are the main driving forces behind the effort to explore properties and practical applications of this fascinating material. Nanotubes can today be grown with very high qualities and at precisely determined locations with lengths already reaching several millimeters. As a consequence of these advances, the focus of experimental work is now slowly shifting towards exploring practical applications and device architectures that would be able to fully profit from the extremely high Young's modulus and flexibility of CNTs, most notably in the fabrication of electromechanical switches and oscillators operating at ever higher frequencies. [22]

Boris I. Yakobson et. al. (2001) This paper presents an overview of the mechanical properties of carbon nanotubes, starting from the linear elastic parameters, nonlinear elastic instabilities and buckling, and the inelastic relaxation, yield strength and fracture mechanisms. A summary of experimental findings is followed by more detailed discussion of theoretical and computational models for the entire range of the deformation amplitudes. Non-covalent forces between the nanotubes and with the substrates are also discussed, due to their significance in potential applications. It is noteworthy that the term resilient was first applied not to nanotubes but to smaller fullerene cages, the very same property of resilience becomes more significant in the case of carbon nanotubes, since their elongated shape, with the aspect ratio close to a thousand,

makes the mechanical properties especially interesting and important due to potential structural applications. [23]

Jin-Liang Zang et. al. (2009) Young's modulus holds the special status in material properties and micro/nano-electromechanical systems (MEMS/NEMS) design. The excellently regular structures of CNTs facilitate accurate simulation of CNTs' behavior by applying a variety of theoretical methods. Here, three representative numerical methods, i.e., Car–Parrinello molecular dynamics (CPMD), density functional theory (DFT) and molecular dynamics (MD), were applied to calculate Young's modulus of single-walled carbon nanotube (SWCNT) with chirality (3,3). The comparative studies showed that the most accurate result is offered by time consuming DFT simulation. MD simulation produced a less accurate result due to neglecting electronic motions. Compared to the two preceding methods the best performance, with a balance between efficiency and precision, was deduced by CPMD. [24]

N. Nouri et. al. (2010) One such application is producing nanotube thin pages called buckypaper. These pages, known as nanotube sheets, have signi_cant physical, chemical, mechanical, thermodynamic and electromagnetic properties, such as being several times stronger than steel. Computer simulations can be used as a powerful tool to discover the mechanical properties of these materials. The aim of the present research is to investigate the mechanical behavior of buckypaper using the nite element method. The molecular network of buckypaper, which consists of a regular arrangement of CNTs, is modeled as a structure with its atoms as nodes, its bonds as 3-D-beam elements and Van der Waals forces by means of nonlinear forces. A computer program is then developed to calculate the mechanical properties of buckypaper especially the modulus of elasticity. In this program, the nanotubes are arranged together to create a simple ordered network with periodic boundary conditions resembling real buckypaper. [25]

John D. Joannopoulos et. al. (2004) proposed a realistic microscopic quantum mechanical description of the properties of real material systems. Theoretical attempts to deduce microscopic electronic and geometric structure had been generally based on optimizing geometry to fit known experimental data. The approach is more fundamental: predicting geometric, electronic, and

dynamical structure, ab-initio that is, given only the atomic numbers of the constituent atoms as experimental input. The method makes it possible to accurately and efficiently calculate the total energy of a solid by the use of density functional theory, pseudo potential theory and a conjugate gradients iterative minimization technique for relaxing the electronic and nuclear coordinates. Ab-initio investigations are invaluable because they make possible theoretical calculations or simulations that can stand on their own. They were complement experimental observations but needed not be guided by experimental interpretations. This paper put forward a fundamental, microscopic understanding of various physical and chemical phenomena of real materials systems. [26]

E. Mohammadpour(2011) proposed a Single Walled Carbon Nanotube (SWCNT) finite element (FE) model, based on the use of nonlinear and torsional spring elements, to evaluate its mechanical properties. The choice of the spring elements to build the FE model was based on the observation that other elements as beam, truss or shell are not very applicable because of the complex interaction of many atoms and the absence of rotational degrees of freedom. Moreover, it was also possible to model the bond interaction without introducing any non-physical variable, such as area and inertia of atoms linkage when using beam elements. [27]

Toshiaki Natsuk et. al.(2003) developed an analytical method was developed for modeling the elastic properties of single-walled carbon nanotubes (SWNTs). A SWNT is regarded as a continuum-shell model which is composed of the discrete molecular structures linked by the carbon-to carbon bonds. The elastic properties were investigated for the SWNTs as a function of the nanotube size in terms of the chiral vector integers m,n The theoretical prediction on elastic properties agreed reasonably with the existing experiment and theoretical results. The present formulas are able to serve as a good approximation of the elastic properties for SWNTs. [28]

Michele Meo et. al.(2006) proposed a Single Walled Carbon Nanotube (SWCNT) finite element (FE) model, based on the use of nonlinear and torsional spring elements, to evaluate its mechanical properties. The choice of the spring elements to build the FE model was based on the observation that other elements as beam, truss or shell are not very applicable because of the complex interaction of many atoms and the absence of rotational degrees of freedom. Moreover,

it was also possible to model the bond interaction without introducing any non-physical variable, such as area and inertia of atoms linkage when using beam elements. [29]

Tao Zhou et. al.(2008) The radial breathing modes (RBMs) of (MgO)*n* and (BeO)*n* rings (*n*=3−10) were calculated using the density functional theory at B3LYP/6-31G(*d*) level. It was found that for large rings, the radial breathing mode (RBM) frequency was inversely proportional to the center diameter, but the variation of bond length may lead to deviations from a linear behavior. The deviations caused by inverse cubic term of diameter and variation of bond length, became dramatic with the decrease of ring diameter. From the point of chemical bond view, using one-dimensional harmonic oscillator and the method of cascade and parallel connection of "springs", the linear relation and deviations were explained. The model can be applied to nanotubes. [30]

S.K. Georgantzinos et. al. (2009) The excellent properties of carbon nanotubes have generated technological interests in the development of nanotube/rubber composites. The paper describes a finite element formulation that is appropriate for the numerical prediction of the mechanical behavior of rubber-like materials which are reinforced with single walled carbon nanotubes. The considered composite material consists of continuous aligned single walled carbon nanotubes which are uniformly distributed within the rubber material. It is assumed that the carbon nanotubes are imperfectly bonded with the matrix. Based on the micromechanical theory, the mechanical behavior of the composite may be predicted by utilizing a representative volume element. Within the representative volume element, the reinforcement is modeled according to its atomistic microstructure. Therefore, non-linear spring-based line elements are employed to simulate the discrete geometrical structure and behavior of the single-walled carbon nanotube. On the other hand, the matrix is modeled as a continuum medium by utilizing solid elements. In order to describe its behavior an appropriate constitutive material model is adopted. Finally, the interfacial region is simulated via the use of special joint elements of variable stiffness which interconnect the two materials in a discrete manner. Using the proposed multi-scale model, the stress–strain behavior for various values of reinforcement volume fraction and interfacial stiffness is extracted. The influence of the single walled carbon nanotube addition within the rubber is clearly illustrated and discussed.

Chapter 3

3.1 Problem Description

The discovery of carbon nanotubes has stimulated considerable experimental and theoretical studies. Various promising applications have been proposed based on their geometrical and mechanical properties. Due to difficulties in experimental investigation of Carbon Nanotubes analytical methods have to be developed. Carbon nanotubes are stimulated extensively using molecular mechanics, tight-bonding molecular dynamics and density. Despite the fact that these approaches can be used for any problem associated with molecular or atomic motions, their huge computational tasks restricted their application to smaller number of molecules or atoms. Since a nanotube can well described as continuum solid beam or shell subjected to tension, bending or torsional forces which means that their mechanical properties of such structure can be obtained by classical continuum model. But due to the uncertainty of the nanotubes characteristics for both the above techniques the obtained mechanical properties of carbon nanotubes are widely scattered.

The main objective is to propose a method to predict mechanical properties of carbon nanotubes. The effect of various parameters of Carbon Nanotubes on their mechanical properties is also discussed.

3.2 Methodology Used

In order to define the Single Walled Carbon Nanotubes mechanical properties, the molecular mechanics theory can be used. According to which molecular mechanics is the mechanics of atomic nuclei moving around, in molecule or in an assembly of molecules. The total force on each nucleus is the sum of the force generated by the electrons and electrostatic force between the positively charged nuclei themselves. The potential energy depends solely on the relative positions of nuclei. The force field being generated from this potential function and acting on the moving nuclei is called the molecular force field. To evaluate such physical quantities, the motion of the whole system under an assumed potential function can be simulated according to the classical or the quantum mechanical equation of motion.

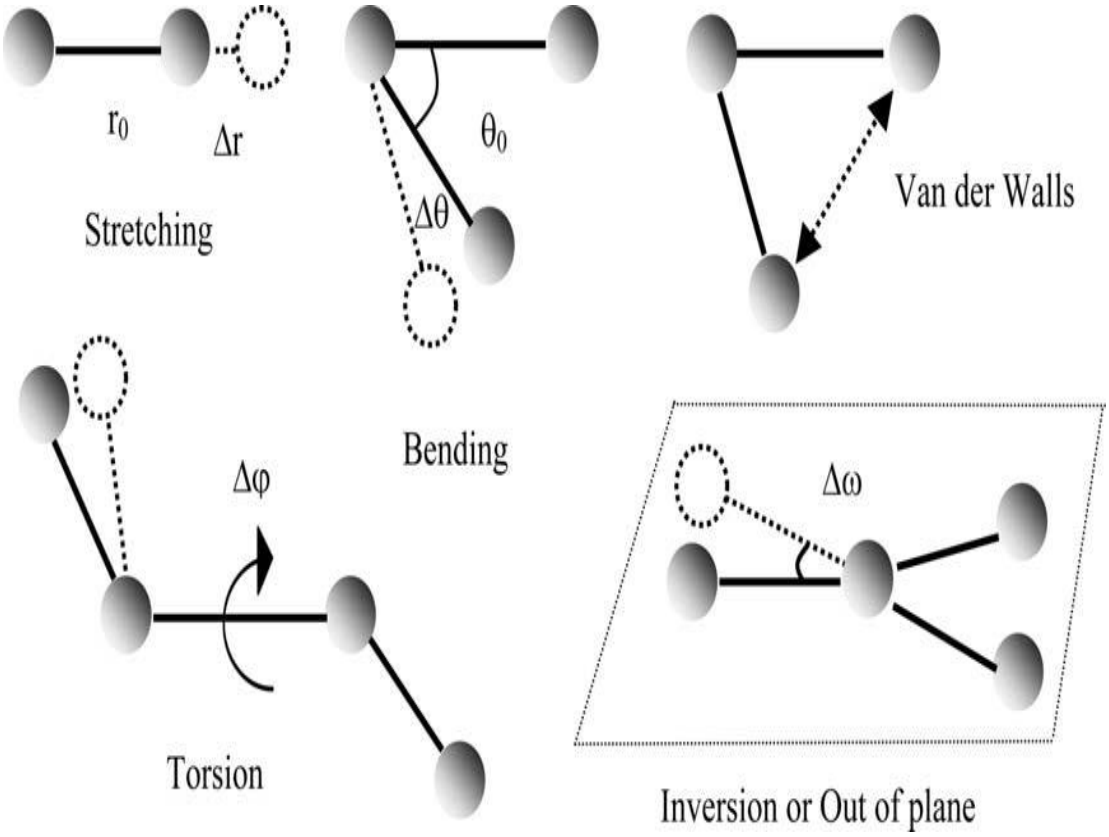

Figure 10: Interatomic interaction in molecular mechanics theory.

In its general formula, the potential energy is described as:

$$V=\sum Vr+\sum V\phi+\sum V\omega+\sum V\theta+\sum Vvdw+\sum Vel$$

Where Vr is the bond stretching, Vϕ is the bond angle bending, Vθ is the dihedral angle torsion, Vw is the inversion terms, Vvdw is the Van der Walls interaction and Vel is the electrostatic interaction. An attempt to represent the experimentally determined bond energy curves of diatomic molecules by simple analytical functions.

$$\mathbf{Vr = (De/S-1)* exp[-\sqrt{(2S)}*\beta*\Delta r]}$$

Where S and β are empirical constants, De is the potential well depth and Δr is the change in bond length.

By deriving the above equation it is possible to have relation force per unit bond length.

$$\mathbf{F(\Delta r) = \sqrt{(2S)}*\beta*[De/(S-1)]*exp[-\sqrt{(2S)}*\beta*\Delta r]}$$

The value of parameters used vary according to the change in bond length i.e. Δr.

3.3 SWCNT Young's Modulus Evaluation

Young's Modulus is the measure of stiffness of an elastic material. It is defined as the ratio of the uniaxial stress over the uniaxial strain.

For calculating the Young's modulus, one nanotube extremity was totally restrained and on the opposite extremity a displacement was imposed. The nanotube Young's modulus was evaluated with the equation:

$$\mathbf{E}young = \frac{Stress}{Strain}$$

$$\mathbf{E} = \frac{\boldsymbol{\sigma}}{\varepsilon}$$

$$= \frac{\boldsymbol{Ftotal/Ao}}{\mathbf{\Delta L/L}o}$$

Where F*total* is the force generated after the displacement imposed

$$\mathbf{A}o = \mathbf{\lrcorner I * D}n\mathbf{*T}n$$

$$\mathbf{D}n = \frac{\boldsymbol{a}o\sqrt{[\mathbf{3}(\boldsymbol{n}^{\mathbf{2}}+\boldsymbol{m}^{\mathbf{2}}+\boldsymbol{nm})]}}{\boldsymbol{\pi}}$$

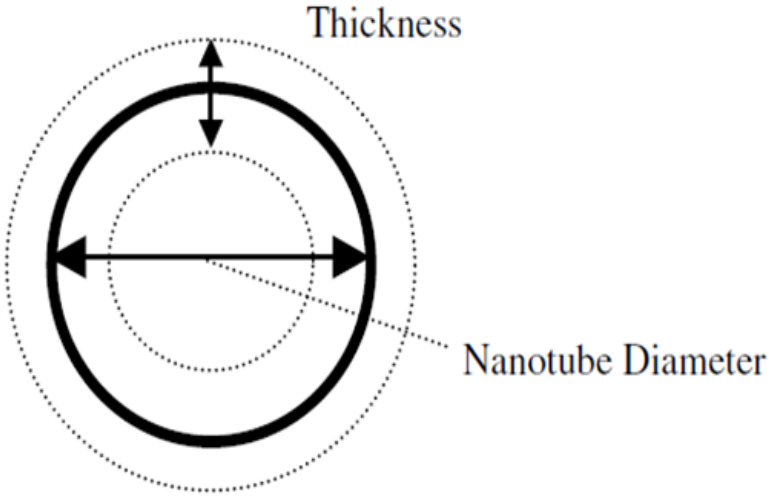

Figure 11: Nanotube top view. Cross sectional area definition.

Where

m,n are the chiral vectors.

ao is the bond length.

D*n* is the nanotube diameter.

T*n* in the thickness of nanotube.

Lo is the nanotube length.

ΔL is the displacement in the length imposed.

Parameters used for the calculation are :

For r = 0.135 nm

De = 6.325 eV

β = 15 nm^{-1}

S = 1.29

For r = 0.139 nm

De = 6.0 eV

β = 21 nm^{-1}

S = 1.22

For r = 0.145

De = 9.64798622 eV

β = 21 nm^{-1}

S = 1.22

Chapter 4

Analysis

4.1 Calculation of Young's Modulus using Rebo Potential

Parameters:

a_o = 0.135 nm

De = 1.01337 * 10^{-9} N-nm

β = 15 nm^{-1}

S = 1.29

Table 3: Calculation of Young's Modulus using Rebo Potential: Parameters 1

m,n	area	Young's Modulus
3,0	**2.38503**	**2.18025**
4,0	**3.18005**	**1.63518**
5,0	**3.97506**	**1.30815**
6,0	**4.7707**	**1.08998**
7,0	**5.56508**	**0.934391**
8,0	**6.36009**	**0.817592**

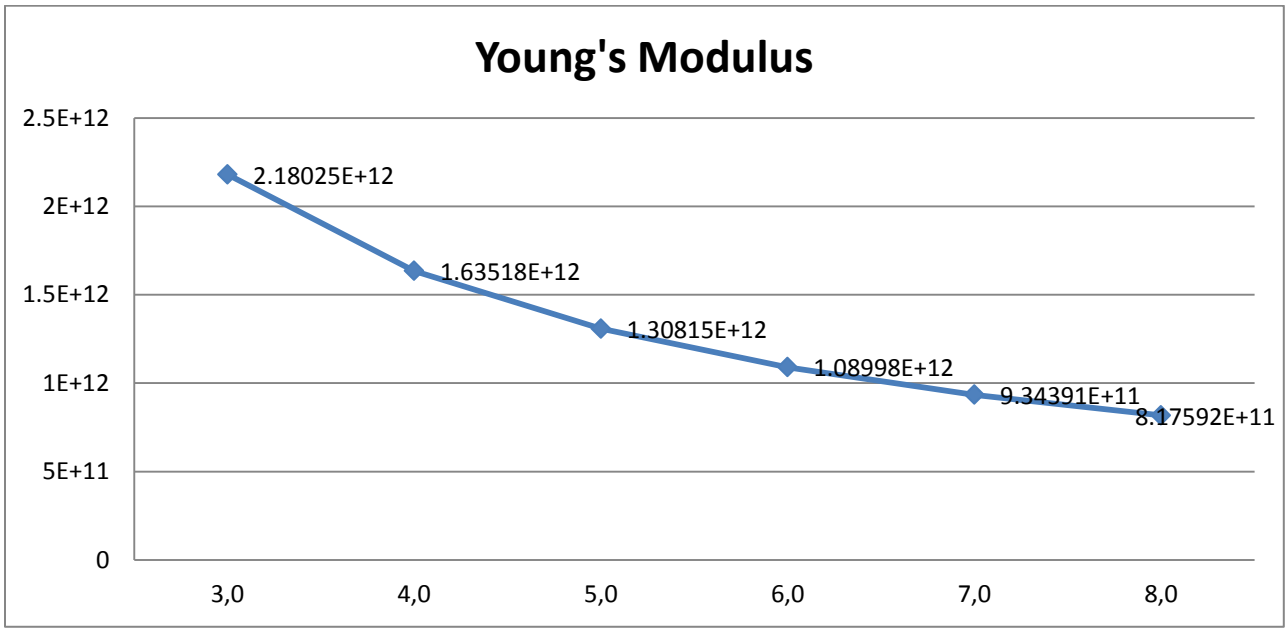

Figure 12: Variation of Young's Modulus with area at a_o=0.135

1. **Parameters:**

a_o = 0.139 nm

De = 9.61305877 * 10^{-9} N-nm

β = 21 nm^{-1}

S = 1.22

Table 4: Calculation of Young's Modulus using Rebo Potential: Parameters 2

m,n	area	Young's Modulus
3,0	2.4557	3.02835
4,0	3.27427	2.27126
5,0	4.09284	1.81701
6,0	4.9114	1.51417
7,0	5.72997	1.29786
8,0	6.54854	1.13563

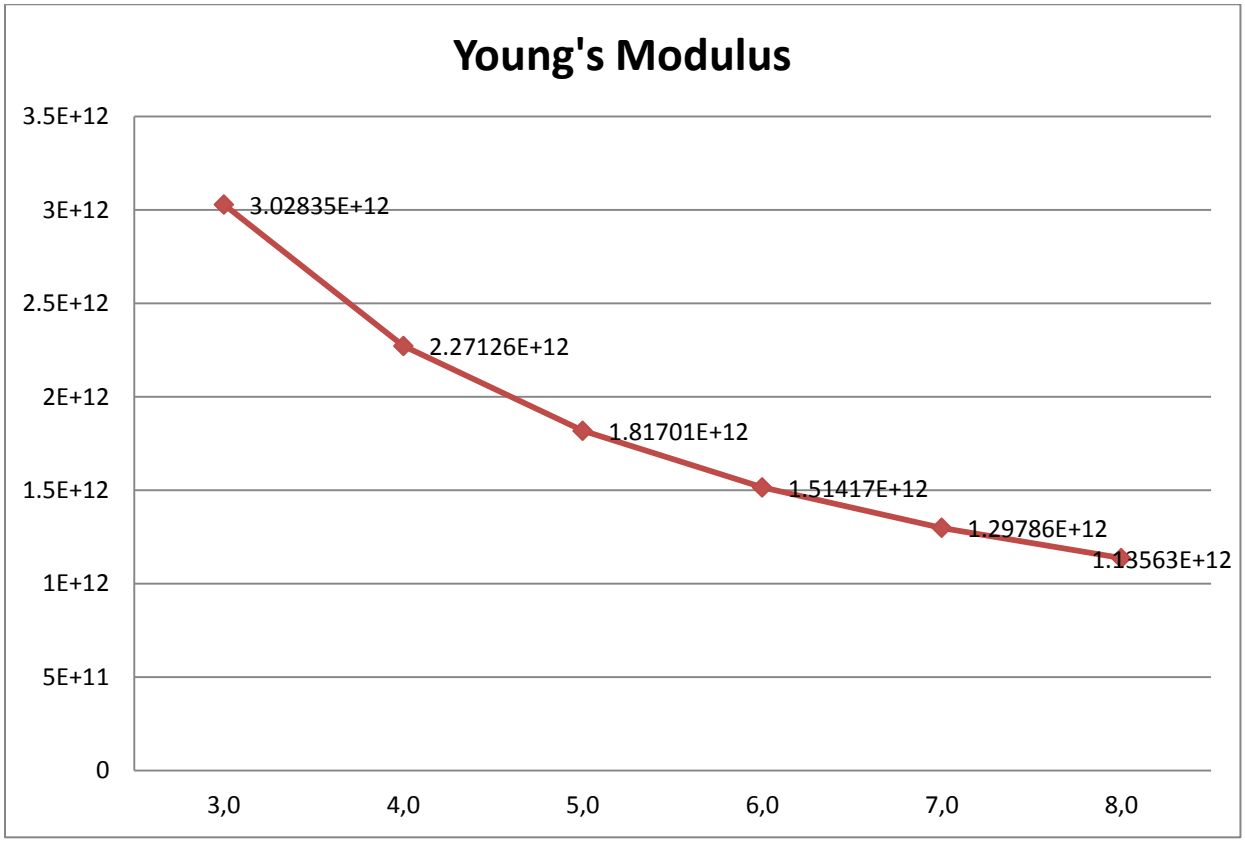

Figure 13: Variation of Young's Modulus with area at a_o = 0.139 nm

Parameters:

a_o = 0.145 nm

De = 9.61305877 * 10^{-9} N-nm

β = 21 nm^{-1}

S = 1.22

Table 5: Calculation of Young's Modulus using Rebo Potential: Parameters 3

m,n	area	Elastic Modulus
3,0	**2.5617**	**2.91392**
4,0	**3.4156**	**2.18544**
5,0	**4.26951**	**1.74834**
6,0	**5.1234**	**1.45696**
7,0	**5.97731**	**1.24882**
8,0	**6.83121**	**1.09272**

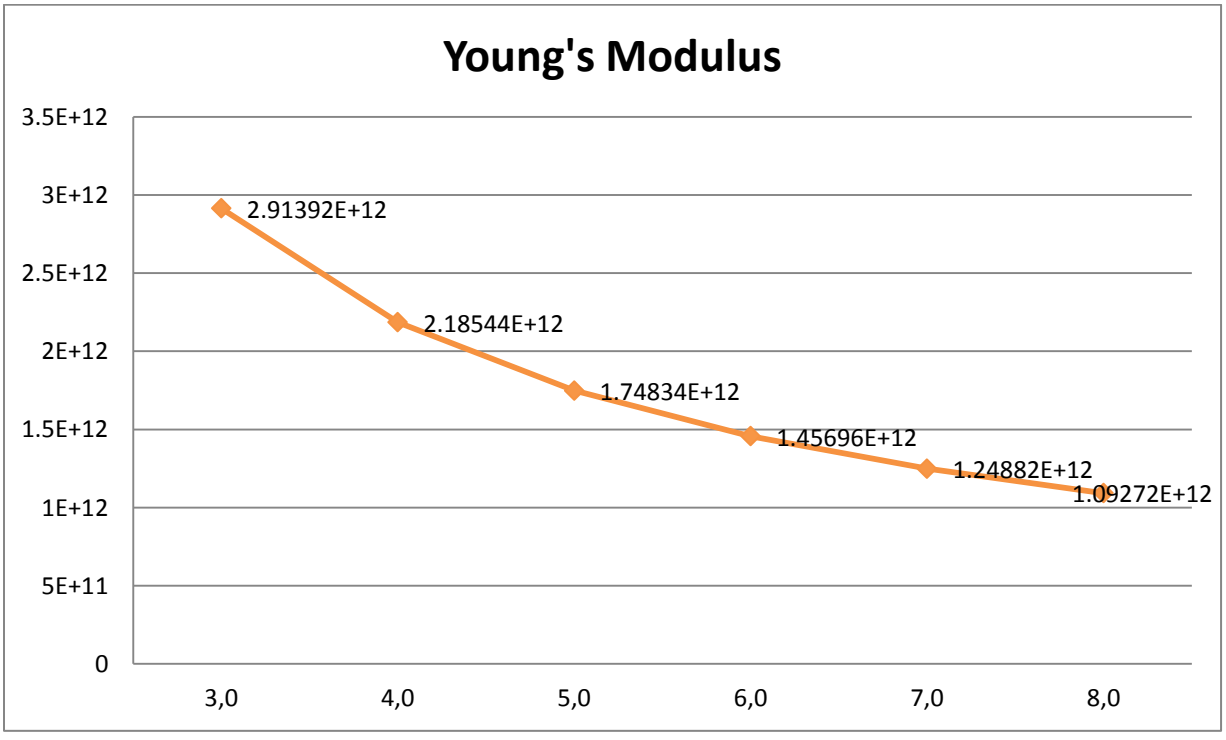

Figure 14: Variation of Young's Modulus with area at a_o = 0.145 nm

4.2 Factors affecting the Young's Modulus

- **Bond Length** - All the parameters used in the equation depends upon the bond length. So a small change in bond length would cause a big change in results obtained. It is the major factor in any type of calculation concerned with Young's Modulus.

Table 6: Calculation of area with different bond lengths

ao, Bond Length	n	m	$D_n = \frac{ao\sqrt{[3(n^2+m^2+nm)]}}{\pi}$	Tn	area=Л*Dn*Tn
0.135	3	0	0.223288391	0.34	0.238503396
0.135	6	0	0.446576782	0.34	0.477006792
0.135	9	0	0.669865174	0.34	0.715510189
0.135	12	0	0.893153565	0.34	0.954013585
0.135	15	0	1.116441956	0.34	1.192516981
0.135	18	0	1.339730347	0.34	1.431020377
0.135	21	0	1.563018739	0.34	1.669523773
0.135	24	0	1.78630713	0.34	1.90802717
0.135	27	0	2.009595521	0.34	2.146530566
0.135	30	0	2.232883912	0.34	2.385033962
0.139	6	0	0.459808687	0.34	0.491140327
0.139	9	0	0.689713031	0.34	0.73671049
0.139	12	0	0.919617374	0.34	0.982280654
0.139	15	0	1.149521718	0.34	1.227850817
0.139	18	0	1.379426061	0.34	1.473420981
0.139	21	0	1.609330405	0.34	1.718991144
0.139	24	0	1.839234749	0.34	1.964561308
0.139	27	0	2.069139092	0.34	2.210131471
0.139	30	0	2.299043436	0.34	2.455701635
0.145	3	0	0.239828272	0.34	0.256170314
0.145	6	0	0.479656544	0.34	0.512340629
0.145	9	0	0.719484816	0.34	0.768510943
0.145	12	0	0.959313088	0.34	1.024681258
0.145	15	0	1.19914136	0.34	1.280851572
0.145	18	0	1.438969632	0.34	1.537021887

- The above table shows the variation in area of nanotube with bond length. Upon changing the bond length a large change in the parameters is observed which results in a large variation in diameter. The diameter change further results in changing the Young's Modulus.
- **Diameter** - Young's Modulus is inversely proportional to diameter of nanotube. With an increase in diameter, The Young's modulus decreases. The value of diameter also depends upon the bond length and the chirality vectors of the nanotube.

$$\textbf{Young's modulus} = \frac{Ftotal/Ao}{\Delta L/Lo}$$

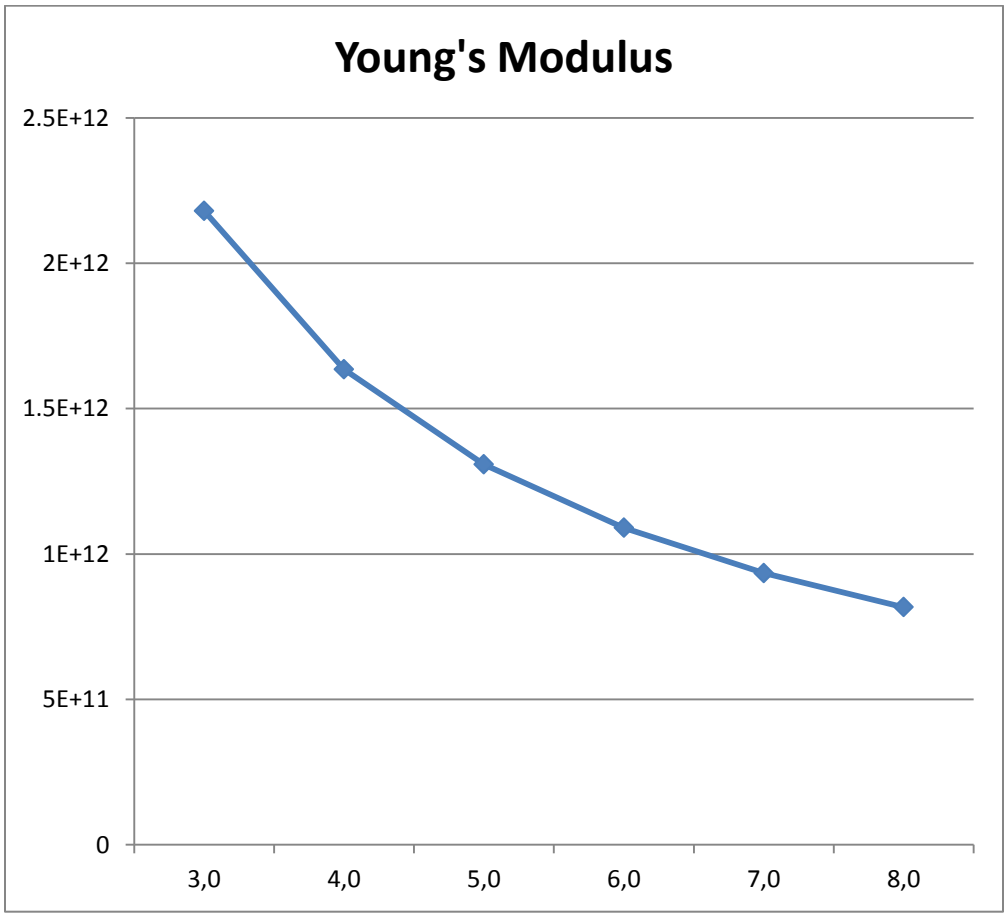

Figure 15: Variation in Young's Modulus with diameter

- **Strain** - The value of Young's Modulus is also varied by varying the strain. A length to radius ratio smaller than 10 could affect the result thus the tests are performed with a ratio

greater, to limit the edge effects. The strain is in inverse proportion with Young's Modulus, which means upon increasing the strain the Young's Modulus would decrease.

Table 7: Length to Diameter ratio for different chiral index

Chiral Index m,n	Diameter Dn	Length of Nanotube	Length to diameter Ratio
5,1	0.436	9.315	21.39
5,2	0.489	10.461	21.67
5,3	0.549	11.781	21.51
5,4	0.612	13.182	21.53
6,5	0.743	16.117	21.54
7,5	0.818	17.684	21.51
8,5	0.889	12.771	14.32
10,5	1.037	11.118	10.72
15,5	1.415	15.213	10.74

4.3 Important Conversions

1 eV = $1.60217*10^{-19}$ Nm

1 nm = 10^{-9} m

1 TPa = 10^{12} Pa

Chapter 5

Results & Discussion

5.1 Results

According to the approach different results are obtained varying certain parameters. The results of this work are in good agreement with numerical and experimental works performed. The calculated value with the approach used, is in agreement with commonly accepted values and with the results of several authors. According to the method an increasing value of Young's modulus is observed with rising value of diameter. According to the Approach 1 the value of Young's Modulus varies from 0.817 to 2.18 TPa. In Approach 2 the values lies in the range from 1.135 to 3.02 TPa and in the Approach 3 the value is in range 1.092 to 2.913 TPa.

Table 8: Result of variation in Young's Modulus for the different approaches

	m,n	3,0	4,0	5,0	6,0	7,0	8,0
Approach 1	0.135	2.18025	1.63518	1.30815	1.08998	0.93439	0.81759
Approach 2	0.139	3.02835	2.27126	1.81701	1.51417	1.29786	1.13563
Approach 3	0.145	2.91392	2.18544	1.74834	1.45696	1.24882	1.09272

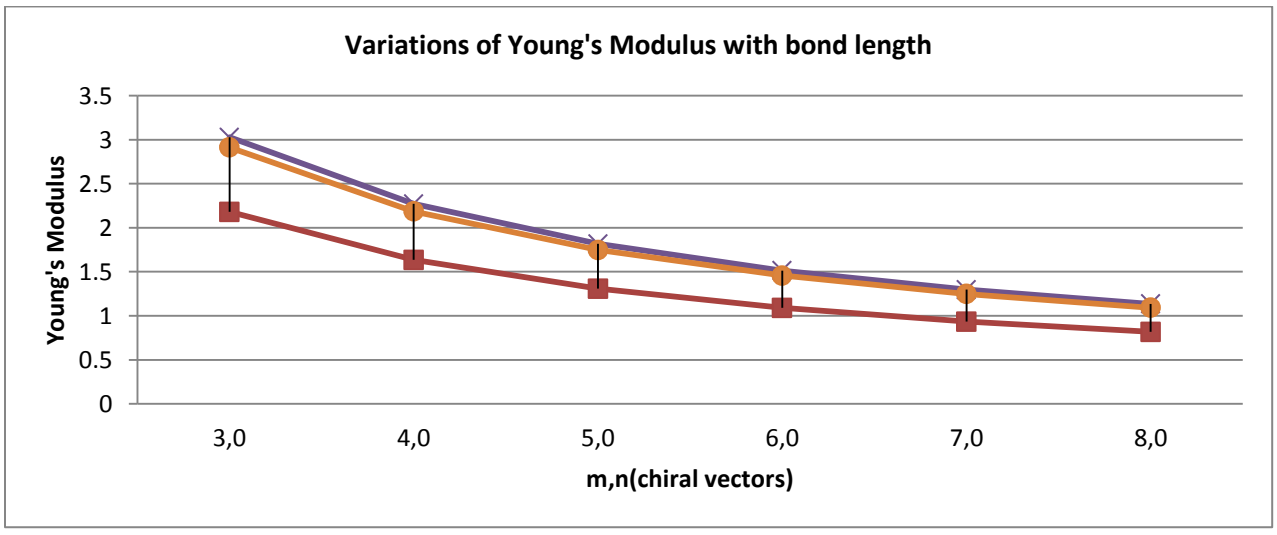

Figure 16: Variation of Young's Modulus for three Different approaches.

5.2 Conclusion

The proposed method is tested on CC bond of several Carbon Nanotubes. The Young's Modulus calculated is in good agreement with several authors. Several carbon nanotubes, with different diameter and chirality, were tested under uniaxial load in order to evaluate their Young's modulus. The results obtained lie in between the range of 0.6 TPa to 5 TPa. Young's Modulus is resistance of material to deform under load. The variation in Young's Modulus is due to certain factors which are bond length, diameter, strain and thickness. Different values of diameter are obtained for different chirality and bond length. Upon increasing the value of diameter the value of Young's Modulus decreases and vice versa.

5.3 Future Scope

Due to difficulties in experimental investigation of Carbon Nanotubes analytical methods have to be developed which can be easily solved and values of mechanical properties can be calculated. Carbon nanotubes are stimulated extensively using molecular mechanics, tight-bonding molecular dynamics and density. Despite the fact that these approaches can be used for any problem associated with molecular or atomic motions, their huge computational tasks restricted their application to smaller number of molecules or atoms.

Following are certain advantages of the new approach:

- It is easier to calculate the Young's Modulus without huge computational tasks.
- With the help of new approach it would be easier to study Variation of elastic modulus with basic parameters of carbon nanotubes.

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References

1. **Aleksander Muc**, "Design and identification methods of effective mechanical properties for carbon nanotubes", Journal of materials and design, 1671–1675, 2010.
2. **P. Zhang, Y. Huang, P.H. Geubelle, P.A. Klein, K.C. Hwang**, "The elastic modulus of single-wall carbon nanotubes: A continuum analysis incorporating interatomic potentials", International Journal of Solids and Structures 39, 3893–3906, 2002.
3. **Dong Qian, Gregory J Wagner, and Wing Kam Liu**, "Mechanics of carbon nanotubes", Journal of American Society of Mechanical Engineers, 2002.
4. **Jean-Paul Salvetat, G. Andrew D. Briggs, Jean-Marc Bonard, Revathi R. Bacsa, Andrzej J. Kulik, Thomas Stöckli, Nancy A. Burnham, László Forró**, "Elastic and Shear Moduli of Single-Walled Carbon Nanotube Ropes", The American Physical Society, 1999.
5. **K.S. Challagulla, A.V. Georgiades, G.C. Saha, A.L. Kalamkarov**, "Micromechanical Analysis of Grid-Reinforced Thin Composite Generally Orthotropic Shells".
6. **T. Belytschko, S.P. Xiao, G.C. Schatz and R. Ruoff**, "Atomistic Simulations of Nanotube Fracture", K. Mylvaganam, L.C. Zhang, "Important issues in a molecular dynamics simulation for characterizing the mechanical properties of carbon nanotubes" , Elsevier journal, Carbon 42, 2025–2032, 2004.
7. **Eric W. Wong, Paul E. Sheehan, Charles M. Lieber**, "Nanobeam Mechanics: Elasticity, Strength, and Toughness of Nanorods and Nanotubes", Science Magzine, vol. 277, 1997.
8. **O. Breuer, Uttandaraman Sundararaj**, "Big Returns from Small Fibers: A Review of Polymer/Carbon Nanotube Composites", Society of Plastics Engineers, 2004.
9. **Mahmoud Nadim Nahas, Mahmoud Abd-Rabou**, "Finite element modeling of carbon nanotubes", International Journal of Mechanical & Mechatronics Vol. 10, 2010.
10. **Pulickel M. Ajayan, Otto Z. Zhou**, "Applications of Carbon Nanotubes", Appl. Phys. 80, 391–425, 2001.
11. **Chunyu Li, Rodney S. Ruoff, Tsu-Wei Chou**, "Modeling of carbon nanotube clamping in tensile tests", Composites Science and Technology 65 (2005) 2407–2415.

12. **Marino Brcic, Marko Canadija, Josip Brnic, Domagoj Lanc, Sanjin Krscanski and Goran Vukelic**' "FE modelling of multi-walled carbon nanotubes", Estonian Journal of Engineering, 2009.
13. **Mehrdad Arjmand, Ali Shokuhfar, Mohammad Amini Sarabi, Hesam Ghourchibeigy**, "A theoretical study to predict the young's modulus of zigzag single walled carbon nanotubes containing vacancies", Journal of Nanocon 2010.
14. **K. Udhaya kumar, P. A. Gowri Sankar**, "Mechanical and Electrical Properties of Single Walled Carbon Nanotubes: A Computational Study", European Journal of Scientific Research, 2011.
15. **Michael Griebel, Jan Hamaekers**, "Molecular Dynamics Simulations of the Elastic Moduli of Polymer-Carbon Nanotube Composites", Elsevier Science, 2004.
16. **A. Zettl, J. Cumings, Wei-qiang Han, W. Mickelson**, "Boron nitride nanotube peapods", Structural and Electronic Properties of Molecular Nanostructures, 2002.
17. **W. Mickelson, S. Aloni, Wei-Qiang Han, John Cumings, A. Zettl**, "Packing C60 in Boron Nitride Nanotubes", Science Magazine, Vol. 300, 2003.
18. **Chung-Jung Wu, Chan-Yen Chou, Cheng-Nan Han, and Kuo-Ning Chiang**, "Simulation and Validation of CNT Mechanical Properties – The Future Interconnection Material", IEEE 2007.
19. **K T Kashyap, R G Patil**, "On Young's modulus of multi-walled carbon nanotubes", Bull. Mater. Sci., Vol. 31, No. 2, April 2008.
20. **Douglas Vodnik, Dr. Kevin Crosby**, "The Young's Modulus of Single-Walled Carbon Nanotubes".
21. **Kaveh Pour Akbar Saffar, Nima JamilPour, Ahmad Raeisi Najafi, Gholamreza Rouhi**, "Finite element model for estimating young's modulus of carbon nanotube reinforced composites incorporating elastic cross-links", International Journal of Aerospace and Mechanical Engineering 2:3, 2008.
22. **Andras Kis, Alex Zettl**, "Nanomechanics of carbon nanotubes", Phil. Trans. R. Soc. A, 1591–1611, 2008.
23. **Boris I. Yakobson, Phaedon Avouris**, "Mechanical properties of carbon nanotubes", Topics Appl. Phys. 80, 287–327, 2001.

24. **Jin-Liang Zang, Quanzi Yuan, Feng-Chao Wang, Ya-Pu Zhao**, "A comparative study of Young's modulus of single-walled carbon nanotube by CPMD, MD and first principle simulations", Computational Materials Science 46, 621–625, 2009.
25. **N. Nouri, S. Ziaei-Rad**, "Mechanical property evaluation of carbon nanotube sheets", Nanotechnology, Vol. 17, No. 2, 2010.
26. **John D. Joannopoulos**, "Ab-initio calculations of materials properties", Phys. Rev. B 69, 035316-1–035316-7, 2004.
27. **E. Mohammadpour, M. Awang, M.Z. Abdullah,** "Predicting the Young's Modulus of carbon nanotubes using finite element modeling.", Journal of Applied Sciences, 1653-1657,2011.
28. **Toshiaki Natsuki, Kriengkamol Tantrakarn, Morinobu Endo, "**Prediction of elastic properties for single-walled carbon nanotubes", Elsevier Science Magazine, Carbon 42 (2004) 39–45.
29. **Michele Meo, Marco Rossi**, "An analytical molecular structural mechanics model for the mechanical properties of carbon nanotubes", International Journal of Solids and Structures 42 (2005) 3075–3092.
30. **Tao Zhou, Can Xu, Xiaofang Zhang, Chuan Cheng, Liang Chen, Ying Xu, "**A simple theoretical model for ring and nanotube radial breathing mode", **Acta Physico-chimica Sinica** volume 24, issue 9, september 2008.