DERIVATION OF FINITE ELEMENT MODELS OF CONNECTED CARBON NANOTUBES WITH HETEROJUNCTIONS

MOJTABA AKBARZADEH

A project report submitted in partial fulfilment of the
requirements for the award of the degree of
Master of Engineering (Mechanical)

Faculty of Mechanical Engineering
Universiti Teknologi Malaysia

JANUARY 2014

DEDICATION

I praise God, the almighty for providing me this opportunity and granting me the capability to proceed this research. I would like to dedicate this dissertation to my beloved parents.

ACKNOWLEDGEMENTS

I praise Allah, continuously, though my fervent does not do justice to His glory.

Foremost, I would like to express my sincere gratitude to my supervisor Professor Dr. Andreas Oechsner for the continuous support of my study and research, for his patience, motivation, enthusiasm, and immense knowledge. His guidance helped me during the time of research and writing of this project report. I could not have imagined having a better advisor and mentor for my Master study.

Besides, I would also like to thank my co-supervisor Professor Dr. Nasir Tamin for his selfless support and constant encouragement. His advices helped me greatly through my project.

Lastly, I would like to thank my friends Aria Enzevaee and Ghasem Ghadyani for all their help through my hard times during the project. I wouldn't have finished this work if it weren't for their help.

ABSTRACT

After the discovery of carbon nanotubes (CNTs) and their considerable applications, scientists have been interested to explore the properties of these outstanding nanomaterials in any field. Due to the different types of CNTs and different methods of analyses, the discovery of mechanical properties of carbon nanotubes are still in progress. One type of CNT which is very applicable in electronic field is one consisting of two connected CNTs with a heterojunction. Heterojunctioned CNTs are connected by an angular or conic junction. Simulation of CNTs in an analysis software is one way to find some of the mechanical properties of CNTs but for modeling of heterojunctions an algorithm should be considered. ConTub is an algorithm as well as online software for modeling these types of CNTs. In this project, different types of CNTs with heterojunction are created in ConTub then imported to MSC.Marc which is an analysis software, and some mechanical properties such as Young’s modulus, shear modulus, buckling behavior and natural frequency are investigated.

ABSTRAK

Selepas penemuan nanotube karbon (CNTs) dan aplikasi besar mereka, ahli-ahli sains telah berminat untuk meneroka sifat-sifat ini nanobahan cemerlang dalam apa jua bidang. Disebabkan oleh pelbagai jenis CNTs dan kaedah yang berbeza analisis , penemuan sifat mekanik nanotube karbon masih dijalankan. Salah satu jenis CNT yang sangat berkenaan dalam bidang elektronik adalah salah satu yang terdiri daripada dua CNTs berkaitan dengan Heterosimpang a. CNTs Heterojunctioned dihubungkan dengan persimpangan sudut atau kon. Simulasi CNTs dalam perisian analisis adalah salah satu cara untuk menemui beberapa sifat-sifat mekanik CNTs tetapi untuk pemodelan heterojunctions algoritma perlu dipertimbangkan. ConTub adalah satu algoritma serta perisian dalam talian untuk model jenis CNTs . Dalam projek ini , pelbagai jenis CNTs dengan Heterosimpang dicipta dalam ConTub kemudian diimport ke MSC.Marc yang merupakan perisian analisis , dan beberapa sifat-sifat mekanikal seperti modulus Young , modulus ricih, lengkokan tingkah laku dan frekuensi semulajadi dikaji.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF SYMBOLS

Å	Angstrom
θ	Angle
v	Poisson ratio
A	Area
J, I_{xx}, I_{yy}	Second moment of inertia
d_{CNT}	Diameter of carbon nanotube
b	Bond length of carbon nanotube
l	Length
$\bar{d}$	Average diameter of heterojunction
η	Aspect ratio of junction
k_θ, k_φ, k_r	Force field constants
E	Young's modulus
G	Shear modulus
R_b	Bond radius
σ	Stress
ε	Longitudinal strain
P_{cr}	Critical load
t	Thickness
τ	Shear stress
γ	Torsional strain
$\bar{m}$	Mass unit per length
f	Frequency

LIST OF ABBREVIATIONS

STM	Scanning tunneling microscope
CNTs	Carbon nanotubes
SWNTs	Single-walled carbon nanotubes
CVD	Chemical vapor deposition
AFM	Atomic force microscopy
TEM	Transmission electron microscope
GPa	Giga Pascal
TPa	Tera Pascal
CNTFETs	Carbon nanotube field-effect transistors
PDB	Protein-data-bank
FE	Finite element
MD	Molecular dynamic
FEM	Finite element method
TB	Tight-binding
ECM	Equivalent-continuum modeling
MSM	Molecular structural mechanics
ACM	Atomistic-continuum model
IMJs	Intramolecular junctions
FEA	Finite element analysis
NEMS	Nanoscale electromechanical systems

vdW	Van der Walls
PDB	Protein Data Bank

CHAPTER 1

INTRODUCTION

1.1 Background of Nanotechnology

Today, in the young field of nanotechnology, scientists and engineers are taking control of atoms and molecules individually, manipulating them and putting them to use with an extraordinary degree of precision. Word of the promise of nanotechnology is spreading rapidly, and the air is thick with news of nanotech breakthroughs. Governments and businesses are investing billions of dollars in nanotechnology R&D, and political alliances and battle lines are starting to form. Public awareness of nanotech is clearly on the rise, too, partly because references to it are becoming more common in popular culture-with mentions in movies, books, video games, and television.

Yet there remains a great deal of confusion about just what nanotechnology is, both among the ordinary people whose lives will be changed by the new science, and among the policymakers who wittingly or unwittingly will help steer its course. The first use of the concepts in 'nano-technology' was in "There's Plenty of Room at the Bottom," (Fanfair, Desai et al. 2007) a talk given by physicist Richard Feynman at an American Physical Society meeting at Caltech on December 29, 1959.

In this famous speech Feynman addressed the research and development of mechanical inventions at the nano scale although manipulation of atoms and molecules wasn't achieved at the time he gave his remarks. The term "nanotechnology" was defined by Tokyo Science University Professor Norio Taniguchi in a 1974 paper as follows: "'Nano-technology' mainly consists of the processing of, separation, consolidation, and deformation of materials by one atom or by one molecule." In the 1980s the basic idea of this definition was explored in much more depth by (Fanfair, Desai et al. 2007), who promoted the technological significance of nano-scale phenomena and devices through speeches and books.

We define nano-science as the study of phenomena and manipulation of materials at atomic, molecular and macromolecular scales, where properties differ significantly from those at a larger scale; and nanotechnologies as the design, characterization, production and application of structures, devices and systems by controlling shape and size at the nanometer scale.

People are interested in the nanoscale (which we define to be from 100 nm down to the size of atoms (approximately 0.2 nm)) because it is at this scale that the properties of materials can be very different from those at a larger scale. The bulk properties of materials often change dramatically with nano ingredients. Composites made from particles of nano-size ceramics or metals smaller than 100 nanometers can suddenly become much stronger than predicted by existing materials-science models. For example, metals with a so-called grain size of around 10 nanometers are as much as seven times harder and tougher than their ordinary counterparts with grain sizes in the hundreds of nanometers.

The properties of materials can be different at the nanoscale for two main reasons: first, nano-materials have a relatively larger surface area when compared to the same mass of material produced in a larger form. This can make materials more chemically reactive (in some cases materials that are inert in their larger form are reactive when produced in their nanoscale form), and affect their strength or electrical properties; second, quantum effects can begin to dominate the behavior of matter at the nanoscale - particularly at the lower end - affecting the optical, electrical and magnetic behavior of materials.

Truly revolutionary nanotechnology products, materials and applications, such as nano-robotics, are years in the future (some say only a few years; some say many years). What qualifies as "nanotechnology" today is basic research and development that is happening in laboratories all over the world. "Nanotechnology" products that are on the market today are mostly gradually improved products (using evolutionary nano-technology) where some form of nanotechnology enabled material (such as carbon nanotubes, nano-composite structures or nanoparticles of a particular substance) or nanotechnology process (e.g. nano-patterning or quantum dots for medical imaging) is used in the manufacturing process.

In their ongoing quest to improve existing products by creating smaller components and better performance materials, all at a lower cost, the number of companies that will manufacture "nano-products" (by this definition) will grow very fast and soon make up the majority of all companies across many industries. Evolutionary nanotechnology should therefore be viewed as a process that gradually will affect most companies and industries. Economist (Berger 2009) at Merrill Lynch tracks a series of historical growth innovations. He argues that growth innovations drive the economy and the stock market and will become the main driving force of next growth cycle in the near future.

These numbers have reached to 1.5 and 3 sigma. Besides total LOS, Red Zone LOS shows an exponential improvement in both short and long-term situations. The sigma level of ED red zone has rapidly increased from 1.6 and 3.1 to 4.4 and 5.9 in short and long-term conditions.

1.1.1 Discovery of Carbon Nanotube

Nanotechnology and nano-science has two major developments; the birth of cluster science and the invention of the scanning tunneling microscope (STM). The synthesis and properties of semiconductor nano-crystals and this led to a fast increasing number of metal and metal oxide nanoparticles and quantum dots. Advances in the tools that now allow atoms and molecules to be examined and probed with great precision have enabled the expansion and development of nano-science and nanotechnologies. This development led to the discovery of fullerenes in 1986 and carbon nanotubes a few years later. Meantime, these two discoveries also led to a fast increasing number of researches in nanotechnology, especially in carbon nanotechnology.

The ability of carbon bonding with itself and with other atoms in endlessly varied combinations of chains and rings forms the basis of the sprawling modern organic chemistry. The two main types of all-carbon crystalline structure are the naturally occurring allotropes diamond and graphite. All attempts of the world's leading synthetic chemists to prepare novel forms of molecular or polymeric carbon came to nothing: the elegant all-carbon structures proposed by Roald Hoffmann, Orville Chapman and others remained firmly in the realm of pure speculation (Harris). Ultimately, the breakthrough, which revolutionized carbon science, came from experiments on clusters formed by the laser vaporization of graphite.

In 1980s, Harry Kroto, of the University of Sussex and Richard Smalley, of Rice University, came together at Rice began the now famous series of experiments on the vaporization of graphite. They were struck to find that C60, as shown in Fig 1.1, was by far the dominant species in the distribution of gas-phase carbon clusters. C60 are spherical molecules about 1 nm in diameter, comprising 60 carbon atoms arranged as 20 hexagons and 12 pentagons: the configuration of a football. The discovery of C60, (H.W.Kroto 1985), had an impact which extended way beyond the confines of academic chemical physics, and marked the beginning of a new era in carbon science (J.Gaggott 1994, H.Aldersey-Williams 1995, H.W.Kroto 1997, R.E.Smalley 1997). Some of the scientists who discovered this, including Harold

Kroto, Robert Curl and Richard Smalley were awarded the 1996 Nobel Prize in Chemistry.

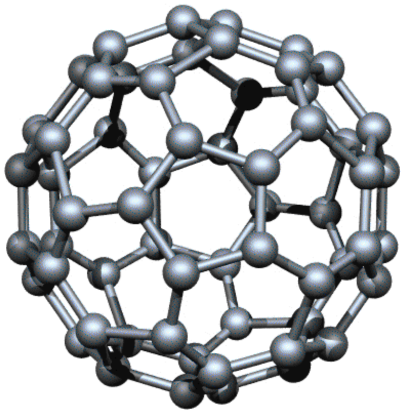

Fig 1.1 Fullerene

The discovery of carbon nanotubes (CNTs) actually originates from fullerenes. The molecules were first discovered by Iijima (S.Iijima 1991), of the NEC laboratories in Japan, in 1991 when he was studying the synthesis of fullerenes by using electric arc discharge technique. Carbon nanotubes that Iijima observed were so called multi-walled carbon nanotubes (MWNTs) as shown in Fig. 1.2a, containing at least two graphitic layers.

Two years later, Iijima and Ichihashi of NEC (D. S. Bethune 1993, S.Iijima 1993) and Bethune and colleagues of the IBM Almaden Research Center in California (IBM 2002) synthesized single-walled carbon nanotubes (SWNTs) as shown in Fig. 1.2b. Since then research on growth and synthesis techniques have been developed to produce nanotubes in sizeable quantities, including arc discharge, laser ablation, high pressure carbon monoxide (HiPCO), and chemical vapor deposition(CVD) (Andrea Szabo 2010). Most of these processes take place in vacuum or with process gases. CVD growth of CNTs can occur in vacuum or at atmospheric pressure. Large quantities of nanotubes can be synthesized by these methods; advances in catalysis and continuous growth processes are making CNTs more commercially viable.

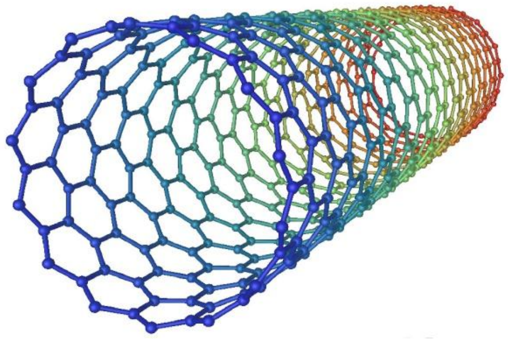

Fig. 1.2b Single walled CNT

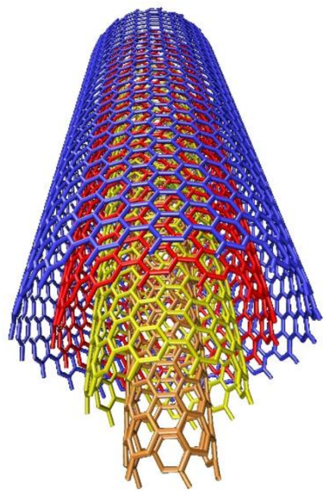

Fig. 1.2a Multi walled CNT

After the discerning and production of CNTs, even broader researches have been stimulated in science and engineering devoted entirely to carbon nanostructures and their applications. Many beautiful images revealing the intricate structure of multi-walled nanotubes caps, internal compartments and so on have been published. Atomic force microscopy (AFM) and scanning tunneling microscopy (STM) have proved more difficult to apply to nanotubes but some useful images (Andrzej Kulik 2004), particularly of single-walled nanotubes, have been achieved recently. Besides transmission electron microscope (TEM) (Z.L.Wang 2000), Raman scattering is perhaps the most widely used characterization technique to study nanotubes.

As a result, we now have a reasonable understanding of the main structural features of both multi-walled and single-walled nanotubes. Already, a broad range of theoretical studies of these hollow concentric graphitic nanotubes has been reported in the literature, focusing their structural properties and mechanical properties. The strong in-plane graphitic carbon - carbon bonds make them exceptionally strong and stiff against axial strains. The almost zero in-plane thermal expansion but large interplane expansion of single walled nanotubes implies strong in-plane coupling and high flexibility against non-axial strains. Meantime, a lot of reviews which provide a comprehensive overview with respect to the synthesis, characterization, applications, and the basic mechanical properties of carbon nanotube have appeared.

Carbon nanotubes have been the center of many researches due to their dimensions and remarkable electro-mechanical properties. Some commercial products on the market today utilizing CNTs include stain resistant textiles, CNT reinforced tennis rackets and baseball bats. Companies like Kraft foods are heavily funding CNT based plastic packaging. Food will stay fresh longer if the packaging is less permeable to atmosphere. Coors Brewing Company has developed new plastic beer bottles that stay cold for longer periods of time. Samsung already has CNT based flat panel displays on the market. A lot of companies are looking forward to being able to produce transparent conductive coatings and phase out ITO coatings. Samsung uses align SWNTs in the transparent conductive layer of their display manufacturing process.

Indeed, NASA is developing materials using nanotubes for space applications, where weight-driven cost is the major concern, by take advantage of their tremendous stiffness and strength. Composites based on nanotubes could offer strength-to-weight ratios beyond any materials currently available. With the advance of materials synthesis and device processing capabilities, the importance of developing and understanding nanoscale engineering devices has dramatically increase over the past decade.

Compared with other nanoscale materials, single-walled carbon nanotubes possess particularly outstanding physical and chemical properties. SWCNTs are remarkably stiff and strong, conduct electricity, and are projected to conduct heat even better than diamond, which suggests their eventual use in nano-electronics. SWCNT are also under intensive study as efficient storage devices, both for alkali ions for nanoscale power sources and for hydrogen for fuel cell applications.

On the other fronts, CNTs also show great potential for biomedical applications due to their biocompatibility and high strength. The current generation of composites used for replacement of bone and teeth are crude admixtures of filler particles that have highly inadequate mechanical properties compared with skeletal tissue. CNTs are also being considered for drug delivery: they could be implanted without trauma at the sites where a drug is needed, slowly releasing a drug over time.

They are also conceivable promise in cellular experiments, where they can be used as nano-pipettes for the distribution of extremely small volumes of liquid or gas into living cells or onto surfaces. It is also conceivable that they could serve as a medium for implantation of diagnostic devices.

1.1.2 Applications of CNTs

1.1.2.1 Structural

Because of the carbon nanotube's superior mechanical properties, many structures have been proposed ranging from everyday items like clothes and sports gear to combat jackets and space elevators. Carbon nanotubes are also a promising material as building blocks in bio-mimetic hierarchical composite materials given their exceptional mechanical properties (~1 TPa in modulus, and ~100 GPa in strength).

1.1.2.2 Electrical Circuits

Nanotube-based transistors, also known as carbon nanotube field-effect transistors (CNTFETs), have been made that operate at room temperature and that are capable of digital switching using a single electron. The first nanotube integrated memory circuit was made in 2004. One of the main challenges has been regulating the conductivity of nanotubes. Depending on subtle surface features a nanotube may act as a plain conductor or as a semiconductor.

1.1.2.3 Electrical Cables and Wires

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

1.1.2.4 Actuators

The exceptional electrical and mechanical properties of carbon nanotubes have made them alternatives to the traditional electrical actuators for both microscopic and macroscopic applications. Carbon nanotubes are very good conductors of both electricity and heat, and they are also very strong and elastic molecules in certain directions.

1.1.2.5 Paper Batteries

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

1.1.2.6 Solar Cells

One of the promising applications of single-walled carbon nanotubes (SWNTs) is their use in solar panels, due to their strong UV/Vis-NIR absorption characteristics.

1.1.2.7 Hydrogen Storage

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

1.1.2.8 Ultra capacitors

MIT Research Laboratory of Electronics uses nanotubes to improve ultracapacitors. The activated charcoal used in conventional ultracapacitors has many small hollow spaces of various size, which create together a large surface to store electric charge. But as charge is quantized into elementary charges, i.e. electrons, and each such elementary charge needs a minimum space, a significant fraction of the electrode surface is not available for storage because the hollow spaces are not compatible with the charge's requirements. With a nanotube electrode the spaces may be tailored to size—few too large or too small—and consequently the capacity should be increased considerably.

1.1.2.9 Radar Absorption

Radars work in the microwave frequency range, which can be absorbed by MWNTs. Applying the MWNTs to the aircraft would cause the radar to be absorbed and therefore seem to have a smaller signature. One such application could be to paint the nanotubes onto the plane.

1.1.2.10 Medical

In the Kanzius cancer therapy, single-walled carbon nanotubes are inserted around cancerous cells, then excited with radio waves, which causes them to heat up and kill the surrounding cells.

1.1.2.11 Optical Power Detectors

A spray-on mixture of carbon nanotubes and ceramic demonstrates unprecedented ability to resist damage while absorbing laser light. Such coatings that absorb as the energy of high-powered lasers without breaking down are essential for optical power detectors that measure the output of such lasers. These are used, for example, in military equipment for defusing unexploded mines. The composite consists of multiwall carbon nanotubes and a ceramic made of silicon, carbon and nitrogen. Including boron boosts the breakdown temperature. The nanotubes and graphene-like carbon transmit heat well, while the oxidation-resistant ceramic boosts damage resistance. Creating the coating involves dispersing he nanotubes in toluene, to which a clear liquid polymer containing boron was added. The mixture was heated to 1,100 ℃ (2,010 ℉). The result is crushed into a fine powder, dispersed again in toluene and sprayed in a thin coat on a copper surface. The coating absorbed 97.5 percent of the light from a far-infrared laser and tolerated 15 kilowatts per square centimeter for 10 seconds. Damage tolerance is about 50 percent higher than for similar coatings, e.g., nanotubes alone and carbon paint.

1.1.2.12 Loud Speaker and Earphone

Carbon nanotubes have also been applied in the acoustics (such as loudspeaker and earphone).

1.2 Problem Statements

The ultimate device miniaturization would be to use individual molecules as functional devices. Single-wall carbon nanotubes are promising candidates for achieving this: depending on their diameter and chirality, they are either one-dimensional metals or semiconductors. Single-electron transistors employing metallic nanotubes and field-effect transistors employing semiconducting nanotubes have been demonstrated. Intramolecular devices have also been proposed which should display a range of other device functions. For example, by introducing a pentagon and a heptagon into the hexagonal carbon lattice, two tube segments with different atomic and electronic structures can be seamlessly fused together to create intramolecular metal-metal, metal-semiconductor, or semiconductor-semiconductor junctions. It is found that a metal-semiconductor junction behaves like a rectifying diode with nonlinear transport characteristics that are strongly asymmetric with respect to bias polarity.

The first computer program for determining the coordinates of heterojunctions between two arbitrary carbon nanotubes have been developed in 2004. This software implements the topological algebra based on the concept of strip, a continuous subset of carbon rings containing all the topological defects (non hexagonal carbon rings). The user easily generates any heterojunction by merely introducing the indices (i,j) and length of the two nanotubes to be connected. The resulting structure is immediately visualized and can be exported in the protein-data-bank (PDB) format. Two classes of heterojunctions are distinguished depending on whether a cone between the connected nanotubes is required. This method is applicable to all kinds of two nanotube heterojunctions, including Dunlap's knees and others related. In addition, this program also generates single and multi-walled carbon nanotubes (SWNT and MWNT).

It is possible to synthesis all configuration of carbon nanotubes but investigation of mechanical properties off all configuration is not possible. For some simple models computational and analytical method can be used. Finite element method is used for complicated models and heterojunction models are categorized in complicated models. Modeling of these carbon nanotubes need to follow an especial algorithm. Contub is an algorithm and also a software for modeling of different configuration of heterojunction which is new and mechanical properties and analysis hetero junction carbon nanotube have not been considered.

In this project, tried to fulfill a numerical method on carbon nanotubes with heterojunction and extract mechanical properties of these types of nanotubes. Procedure of all steps such as software, modeling and analyze are presented in chapter 3 and 4 in detail.

1.3 Research Objectives

The objective of this research is to develop a molecular mechanics based three dimensional finite element model of carbon nanotubes with heterojunctions that facilitates the evaluation of the mechanical properties of carbon nanotubes with heterojunctions under mechanical tests. For this purpose, the following sub-objectives need to be accomplished:

1. To create a tool for automatized generation of finite element model of carbon nanotube with heterojunctions.

2. To develop a three dimensional finite element (FE) model of carbon nanotubes with heterojunctions based on molecular mechanics by applying data transfer between two software programs

3. To evaluate the mechanical properties of the created models including Young's modulus and shear modulus, and compare the results of the proposed FE model with previous ones.

4. To analyze the effect of different diameter and different connection configurations of two carbon nanotubes on young's modulus, shear modulus, critical load on buckling test and natural frequency to compare with the perfect model with the same configuration.

1.4 Research Scope

The following represent the scope of the undertaken project:

1. Literature research on carbon nanotubes with heterojunction

2. Application of the 'nanotube modeler' software to generate coordinates of the carbon nanotubes.

3. Using 'MSC.Marc' finite element software to analyze the models.

4. Applying mechanical tests on the heterojunction models.

5. To characterize the properties of two connected carbon nanotubes by simulating their molecular structures using the finite element method.

It is essential to conduct a profound research into the previous works by other researchers on the subject area in order to acquire the knowledge needed in the field. The next chapter presents the literature review.

1.5 Organization of Project Report

To give a brief idea of how this thesis is organized, the structure of the thesis is listed below.

Chapter 1, the current chapter, talks about the topic and objective of this research with an introduction to CNTs.

Chapter 2 presents a literature study on the past research and some results related to this topic using various approaches.

Chapter 3 talks about the methodology of this research in modeling and evaluating the elastic and properties of CNT with heterojunction. A brief introduction on molecular dynamic (MD), continuum mechanics, fundamentals and formulation of finite element method (FEM) is also presented.

Chapter 4 discusses the results obtained from models developed in Chapter 3 and successful validation is obtained using analytical approaches.

Chapter 5 provides briefly conclusions and discussion on future work.References are collected at the end of this thesis.

REFERENCES

Andrea Szabo, C. P., Anita Csato, Girolamo Fiordano, Danilo Vuono, Janos B.Nagy (2010). Synthesis Methods of Carbon Nanotubes and Related Materials.

Andrzej Kulik, A. K., Gerard Gremaud, Stefan Hengsberger, Philippe Zysset, Laslo Foro (2004). HANDBOOK OF NANOTECHNOLOGY, Springer.

Arghavan, S. and A. Singh (2011). "On the vibrations of single-walled carbon nanotubes." Journal of Sound and Vibration **330**(13): 3102-3122.

Aydogdu, M. (2012). "Axial vibration analysis of nanorods (carbon nanotubes) embedded in an elastic medium using nonlocal elasticity." Mechanics Research Communications **43**: 34-40.

Berger, M. (2009). Nano-society: Pushing the Boundaries of Technology, Royal Society of Chemistry.

Bideau, N., L. Le Marrec and L. Rakotomanana (2011). "Influence of a finite strain on vibration of a bounded Timoshenko beam." International Journal of Solids and Structures **48**(16): 2265-2274.

Cai, J., C. Wang, T. Yu and S. Yu (2009). "Wall thickness of single-walled carbon nanotubes and its Young's modulus." Physica Scripta **79**(2): 025702.

Chang, T., G. Li and X. Guo (2005). "Elastic axial buckling of carbon nanotubes via a molecular mechanics model." Carbon **43**(2): 287-294.

Cheng, H.-C., Y.-L. Liu, Y.-C. Hsu and W.-H. Chen (2009). "Atomistic-continuum modeling for mechanical properties of single-walled carbon nanotubes." International Journal of Solids and Structures **46**(7): 1695-1704.

D. S. Bethune, e. a. (1993). Nature.

Davoudabadi, M., R. Ebrahrmi Naghani and A. Fereidoon (2010). "Prediction of Young's Modulus of Carbon Nanotube Reinforced Composites in Axial Direction with Nonlinear Springs." World Applied Sciences Journal **10**(9): 1007-1019.

Ding, H., S. Chen and K. Cheng (2007). "The atomic-scale finite-element modelling of single-walled carbon nanotubes." Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science **221**(5): 613-617.

Dresselhaus, M. and R. Saito (1995). "Physics of carbon nanotubes." Carbon **33**(7): 883-891.

Ebbesen, T. W. (1997). Carbon nanotubes: preparartion and properties, CRC press.

Ebrahim Zadeh, Z., M. Yadollahpour, S. Ziaei-Rad and F. Karimzadeh (2012). "The effect of vacancy defects and temperature on fundamental frequency of single walled carbon nanotubes." Computational Materials Science **63**: 12-19.

Elements, B. A. o. (2008). "Biological Abundance of Elements, The Internet Encyclopedia of Science." from http://www.daviddarling.info/encyclopedia/E/elbio.html.

Fakhrabadi, M. M. S., A. Amini and A. Rastgoo (2012). "Vibrational properties of two and three junctioned carbon nanotubes." Computational Materials Science **65**(0): 411-425.

Fakhrabadi, M. M. S., A. Amini and A. Rastgoo (2012). "Vibrational properties of two and three junctioned carbon nanotubes." Computational Materials Science **65**: 411-425.

Fakhrabadi, M. M. S., N. Khani, R. Omidvar and A. Rastgoo (2012). "Investigation of elastic and buckling properties of carbon nanocones using molecular mechanics approach." Computational Materials Science **61**: 248-256.

Fanfair, D., S. Desai and C. Kelty (2007). "The early history of nanotechnology." Nanotechnology: Content and Context.

Filiz, S. and M. Aydogdu (2010). "Axial vibration of carbon nanotube heterojunctions using nonlocal elasticity." Computational Materials Science **49**(3): 619-627.

Firmino da Costa, A. (2008). Sociedade de bairro: dinâmicas sociais da identidade cultural, Celta Editora.

Georgantzinos, S., G. Giannopoulos and N. Anifantis (2009). "An efficient numerical model for vibration analysis of single-walled carbon nanotubes." Computational Mechanics **43**(6): 731-741.

Ghavamian, A. and A. Öchsner (2012). "Numerical investigation on the influence of defects on the buckling behavior of single-and multi-walled carbon nanotubes." Physica E: Low-dimensional Systems and Nanostructures.

Ghavamian, A. and A. Öchsner (2013). "Numerical Modeling of the Eigenmodes and Eigenfrequencies of Carbon Nanotubes under the Influence of Defects." Journal of Nano Research **21**: 159-164.

Ghavamian, A. and M. Rahmandoust (2012). "On the determination of the shear modulus of carbon nanotubes." Composites Part B: Engineering.

Ghavamian, A., M. Rahmandoust and A. Öchsner (2013). "On the determination of the shear modulus of carbon nanotubes." Composites Part B: Engineering **44**(1): 52-59.

H.Aldersey-Williams (1995). The most beautiful molecule. London, Aurum Press.

H.W.Kroto, J. R. H., S.C.O'Brien, R.F.Smalley (1985). nature.

H.W.Kroto, J. R. H., S.C.O'Brien, R.F.Smalley (1997). Rec. Mod. Phys.

.

Harris, P. Carbon Nanotubes and Related Structures: New Materials for the Twenty-first Century. 1999, Cambridge University Press, Cambridge.

Hernandez, E., C. Goze, P. Bernier and A. Rubio (1998). "Elastic Properties of C and B_ {x} C_ {y} N_ {z} Composite Nanotubes." Physical Review Letters **80**(20): 4502.

IBM. (2002). "IBM." from http://www. almaden. ibm. com/st/past_projects/nanotubes/

Iijima, S., C. Brabec, A. Maiti and J. Bernholc (1996). "Structural flexibility of carbon nanotubes." The Journal of chemical physics **104**: 2089.

J.Gaggott (1994). Perfect symmetry: the accidental discovery of buckminsterfullerene, Oxford University Press.

Kalamkarov, A. L., A. Georgiades, S. Rokkam, V. Veedu and M. Ghasemi-Nejhad (2006). "Analytical and numerical techniques to predict carbon nanotubes properties." International Journal of Solids and Structures **43**(22): 6832-6854.

Kang, Z., M. Li and Q. Tang (2010). "Buckling behavior of carbon nanotube-based intramolecular junctions under compression: Molecular dynamics simulation and finite element analysis." Computational Materials Science **50**(1): 253-259.

Kinoshita, Y., M. Murashima, M. Kawachi and N. Ohno (2013). "First-principles study of mechanical properties of one-dimensional carbon nanotube intramolecular junctions." Computational Materials Science **70**(0): 1-7.

Kirtania, S. and D. Chakraborty (2007). "Finite element based characterization of carbon nanotubes." Journal of Reinforced Plastics and Composites **26**(15): 1557-1570.

Krishnan, A., E. Dujardin, T. Ebbesen, P. Yianilos and M. Treacy (1998). "Young's modulus of single-walled nanotubes." Physical Review B **58**(20): 14013.

Lau, A. K.-T. and D. Hui (2002). "The revolutionary creation of new advanced materials—carbon nanotube composites." Composites Part B: Engineering **33**(4): 263-277.

Li, C. and T.-W. Chou (2003). "Elastic moduli of multi-walled carbon nanotubes and the effect of van der Waals forces." Composites Science and Technology **63**(11): 1517-1524.

Li, C. and T.-W. Chou (2003). "A structural mechanics approach for the analysis of carbon nanotubes." International Journal of Solids and Structures **40**(10): 2487-2499.

Li, M., Z. Kang, P. Yang, X. Meng and Y. Lu (2013). "Molecular dynamics study on buckling of single-wall carbon nanotube-based intramolecular junctions and influence factors." Computational Materials Science **67**(0): 390-396.

Liu, Y. and X. Chen (2003). "Evaluations of the effective material properties of carbon nanotube-based composites using a nanoscale representative volume element." Mechanics of materials **35**(1): 69-81.

Lu, J.-n. and H.-b. Chen (2008). "Analysis of single-walled carbon nanotubes using a chemical bond element model." Chinese Journal of Chemical Physics **21**(4): 353.

Lu, J. P. (1997). "Elastic properties of carbon nanotubes and nanoropes." Physical Review Letters **79**(7): 1297.

Melchor, S. and J. A. Dobado (2004). "CoNTub: An Algorithm for Connecting Two Arbitrary Carbon Nanotubes." Journal of Chemical Information and Computer Sciences **44**(5): 1639-1646.

Meo, M. and M. Rossi (2006). "Tensile failure prediction of single wall carbon nanotube." Engineering Fracture Mechanics **73**(17): 2589-2599.

Meo, M. and M. Rossi (2007). "A molecular-mechanics based finite element model for strength prediction of single wall carbon nanotubes." Materials Science and Engineering: A **454**: 170-177.

Odegard, G. M., T. S. Gates, L. M. Nicholson and K. E. Wise (2002). "Equivalent-continuum modeling of nano-structured materials." Composites Science and Technology **62**(14): 1869-1880.

Parvaneh, V., M. Shariati and A. M. Majd Sabeti (2009). "Investigation of vacancy defects effects on the buckling behavior of SWCNTs via a structural mechanics approach." European Journal of Mechanics-A/Solids **28**(6): 1072-1078.

Parvaneh, V., M. Shariati and H. Torabi (2011). "Frequency analysis of perfect and defective SWCNTs." Computational Materials Science **50**(7): 2051-2056.

Poncharal, P., Z. Wang, D. Ugarte and W. A. de Heer (1999). "Electrostatic deflections and electromechanical resonances of carbon nanotubes." Science **283**(5407): 1513-1516.

Przemieniecki, J. S. (1963). "Matrix structural analysis of substructures." AIAA Journal **1**(1): 138-147.

Qin, Z., Q.-H. Qin and X.-Q. Feng (2008). "Mechanical property of carbon nanotubes with intramolecular junctions: Molecular dynamics simulations." Physics Letters A **372**(44): 6661-6666.

R.E.Smalley (1997). Rec. Mod. Phys.

Rahmandoust, M. and A. Öchsner (2012). "Buckling Behaviour and Natural Frequency of Zigzag and Armchair Single-Walled Carbon Nanotubes." Journal of Nano Research **16**: 153-160.

Richon, A. B. (1994). "An introduction to molecular modeling." Mathematech **1**: 83.

Rossi, M. and M. Meo (2009). "On the estimation of mechanical properties of single-walled carbon nanotubes by using a molecular-mechanics based FE approach." Composites Science and Technology **69**(9): 1394-1398.

Ru, C. (2000). "Effective bending stiffness of carbon nanotubes." Physical Review B **62**(15): 9973.

S.Iijima (1991). Nature.

S.Iijima (1993). Nature.

Salvetat, J.-P., G. A. D. Briggs, J.-M. Bonard, R. R. Bacsa, A. J. Kulik, T. Stöckli, N. A. Burnham and L. Forró (1999). "Elastic and shear moduli of single-walled carbon nanotube ropes." Physical Review Letters **82**(5): 944.

Scarpa, F. and S. Adhikari (2008). "A mechanical equivalence for Poisson's ratio and thickness of C–C bonds in single wall carbon nanotubes." Journal of Physics D: Applied Physics **41**(8): 085306.

Sun, X. and W. Zhao (2005). "Prediction of stiffness and strength of single-walled carbon nanotubes by molecular-mechanics based finite element approach." Materials Science and Engineering: A **390**(1): 366-371.

Tan, H., L. Jiang, Y. Huang, B. Liu and K. Hwang (2007). "The effect of van der Waals-based interface cohesive law on carbon nanotube-reinforced composite materials." Composites Science and Technology **67**(14): 2941-2946.

Timoshenko, S. (1951). "JN Goodier Theory of elasticity." New York, McGraw-Hill **5**: 50o.

Tirupathi, R. C. and D. B. Ashok (1997). "Introduction to finite elements in engineering." Prentice-Hall, Upper Saddle River, NJ.

To, C. W. (2006). "Bending and shear moduli of single-walled carbon nanotubes." Finite Elements in Analysis and Design **42**(5): 404-413.

Treacy, M., T. Ebbesen and J. Gibson (1996). "Exceptionally high Young's modulus observed for individual carbon nanotubes."

Tserpes, K. and P. Papanikos (2005). "Finite element modeling of single-walled carbon nanotubes." Composites Part B: Engineering **36**(5): 468-477.

Valavala, P., T. Clancy, G. Odegard and T. Gates (2007). "Nonlinear multiscale modeling of polymer materials." International journal of solids and structures **44**(3): 1161-1179.

Viet, N. and W. Kuo (2012). "Load transfer in fractured carbon nanotubes under tension." Composites Part B: Engineering **43**(2): 332-339.

Wang, Y., X.-x. Wang, X.-g. Ni and H.-a. Wu (2005). "Simulation of the elastic response and the buckling modes of single-walled carbon nanotubes." Computational Materials Science **32**(2): 141-146.

Wong, C. and V. Vijayaraghavan (2012). "Nanomechanics of imperfectly straight single walled carbon nanotubes under axial compression by using molecular dynamics simulation." Computational Materials Science **53**(1): 268-277.

Wong, E. W., P. E. Sheehan and C. M. Lieber (1997). "Nanobeam mechanics: elasticity, strength, and toughness of nanorods and nanotubes." Science **277**(5334): 1971-1975.

Xiao, J. R., B. A. Gama and J. W. Gillespie Jr (2005). "An analytical molecular structural mechanics model for the mechanical properties of carbon nanotubes." International Journal of Solids and Structures **42**(11–12): 3075-3092.

Yakobson, B. I., C. Brabec and J. Bernholc (1996). "Nanomechanics of carbon tubes: instabilities beyond linear response." Physical review letters **76**(14): 2511-2514.

Yanovsky, Y. G., E. Nikitina, Y. N. Karnet and S. Nikitin (2010). "Simulation of deformation and fracture of graphene: effect of size, defects and surface modification." Physical Mesomechanics **13**(5): 329-336.

Yao, X., Q. Han and H. Xin (2008). "Bending buckling behaviors of single- and multi-walled carbon nanotubes." Computational Materials Science **43**(4): 579-590.

Yengejeh, S. I., M. A. Zadeh and A. Öchsner (2013). "On the buckling behavior of connected carbon nanotubes with parallel longitudinal axes." Applied Physics A: 1-10.

Z.L.Wang, P. P., W.A.de Heer (2000). Measuring physical and mechanical properties of individual carbon nanotubes by in situ TEM.

Zhao, X. and P. T. Cummings (2006). "Molecular dynamics study of carbon nanotube oscillators revisited." The Journal of chemical physics **124**: 134705.

Zhou, G., W. Duan and B. Gu (2001). "First-principles study on morphology and mechanical properties of single-walled carbon nanotube." Chemical Physics Letters **333**(5): 344-349.