FEM Modeling of Single Walled Carbon Nanotube

A Thesis Submitted for Partial Fulfilment
Of the Requirements for the degree of

Bachelor of Technology
in

Mechanical Engineering
by

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Rourkela-769008
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Under the Supervision of
Dr. Subrata Kumar Panda

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National Institute of Technology, Rourkela,Odisha,769008

CERTIFICATE

This is to certify that the work in this project entitled "FEM Modeling of Carbon Nanotube" by Ram Prasad Parida, has been completed under my watch in partial fulfillment of the necessities for the degree of Bachelor of Technology in Mechanical Engineering amid session 2014-2015 in the Department of Mechanical Engineering, National Institute of Technology, Rourkela.

To the best of my insight, this work has not been submitted to whatever other University/Institute for the recompense of any degree or recognition.

Dr. Subrata Kumar Panda

(Supervisor)

Assistant Professor

Department of Mechanical Engineering

Acknowledgment

I, would take this chance to thank every single person who has helped me to finish this task effectively. To begin with, I might want to express my ardent appreciation to my regarded project guide **Dr. Subrata Kumar Panda**, Assistant Professor (Department of Mechanical Engineering, NIT Rourkela) for his precious direction, inspiration and consistent motivation. His ever co-working state of mind empowered me in raising this proposition in present rich structure. I am truly grateful to **Ajay Kumar**, **Pankaj Katariya**, Department of Mechanical Engineering (M Tech. and Ph.D. scholar) for giving a wide range of conceivable help and exhortation throughout this work.

It is an awesome delight for me to recognize and express my appreciation to my guardians for their understanding, unstinted backing and interminable support amid my study. Finally, I am truly grateful to all the staff members of the department and all my well-wishers, class mates and friends for their inspiration and valuable suggestions.

Submitted by:

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CONTENTS

ABSTRACT

Carbon nanotubes show exceptionally high stiffness, tensile strength, and resilience, which have the potential to be an ideal reinforcement for new Nanocomposites. But before that, research in this field is needed to confirm the use of CNTs in various composites for real world applications. It is very difficult to compute different material properties of these Nano-scale materials. Compared to physical experimentation, Molecular Dynamics (MD) simulation and continuum mechanics model an effective way to model its different properties. The continuum approach has the advantage of analyzing large-scale models over MD simulation. In the present work, modeling of CNT is done through both Finite Element Method (FEM) & MD simulation technique that are two major and distinct research fields. MD Simulation method is used through LAMMPS (Large Atomic Molecular Massively Parallel Simulator) software to evaluate the Young's modulus (superior mechanical property) of CNT. The finite element (FE) model is based on the RVE (Representative Volume Element) technique through ANSYS. This work involves the calculation of one of the important mechanical property (Young's modulus) of a composite where CNT is used as a layer to improve the overall mechanical property of it. The simulation method first develops an armchair structure of CNT, then with the help of accurate coding and potential file, evaluates this property. After getting Young's modulus value of the CNT by simulation technique, Carbon Nanotube is used as homogeneous and isotropic material layer inside a 3-D solid model of the composite matrix. Numerical results from the deformation response of CNT are analyzed to confirm the increment in load carrying capacity of the matrix by the use of CNT layer.

LIST OF FIGURES

LIST OF TABLES

NOMENCLATURE

c_h – Chiral vector

a_1, a_2 – Basis vectors

m, n – Lattice Translational Indices

Θ – Chiral angle

L - Length of matrix element

a - Half of width of matrix element

r_0 – Outter radius

r_i – Inner radius

E_t – Young's modulus of CNT

E_m – Young's modulus of matrix element

μ_t – Poisson's ratio of CNT

μ_m – Poisson's ratio of matrix element

ε_{avg} – Average strain along Z-Direction

V^t – Volume fraction of CNT

CHAPTER 1

INTRODUCTION

1.1 Composites and Nano composites

Composite materials are engineering materials produced by using two or more constituent materials with mainly distinctive physical or chemical properties that stay separate and particular on a macroscopic level within the finished structure. Commonly materials with remarkable contrasts in physical and synthetic properties are picked for a mixture. This aid in acquiring a material that is dominant in qualities from the individual constituents of the mixture. A composite gives a mix of desired properties collected from different constituent components and consequently finds more ease of use than the individual components. Whereas a Nano composite is a solid material where one of the phases has one, two or three dimensions or structures. Nanocomposites vary from the ordinary composite material because of the unusually large surface to volume proportion or excellent aspect ratio.

1.2 Carbon nanotube

Carbon Nanotubes are allotropic forms of carbon with a hollow cylinder or tube-like nanostructure. There are different techniques for synthesis of Carbon nanotubes that include arc discharge, high-pressure carbon monoxide disproportionation, laser ablation, and chemical vapor deposition (CVD). Nanotubes are characterized by high length to diameter proportion (132,000,000:1) which is considerably more than whatever other material. Nanotubes are hollow cylinders with diameters ranging from 1 nm to 50 nm and length over 10µ. They comprised of only carbon atoms and constructed by rolling a graphene sheet into a seamless cylinder typically capped at the ends of half dome shaped fullerene molecules. Nanotubes have raised more interest in modern day research field because of their excellent physical properties. The application of these carbon Nanotubes includes a range from mechanical to the electronic field. For example; the outstanding mechanical properties of carbon nanotubes are beginning to find applications in a whole range of areas, from sports equipment to automobiles.

CHAPTER 2

LITERATURE REVIEW

2.1 LITERATURE REVIEW

Since the revelation of carbon Nanotube by Iijima [1], researchers put their most extreme endeavors to find its different properties. Carbon Nanotubes find a wide range of applications in physics and engineering. However, because of its Nano size carbon nanotubes are still a mystery that prevents from physical tests. Analysts tried to find the properties of single-walled and multi-walled carbon nanotube properties, this lead into many theories regarding carbon nanotubes and followed by the many results regarding the same parameter. Few of researchers even attempted experimental investigation to observe the modulus of single-walled carbon nanotube (SWCNT) lies in a range that is more superior to other composite materials. Krishnan et al. [2] utilized Transmission Electron Microscope (TEM) and observed the vibration of SWCNT and obtained the Young's modulus ranged from 0.90 to 1.70TPa. M. Zakeri et al. [3] conducted FEM Modeling of chiral Nanotubes to model the mechanical properties and concluded with Young's modulus value of 0.93-1.02 Tpa. The Molecular Dynamics (MD) simulation method was used by Griebel and Hamaekers [4] to model mechanical Properties of Polyethylene-Carbon Nanotube Composites. Based on this simulation method reinforcement of the matrix studied and the resulting Young's modulus calculated using a different rule of mixtures.

The uncertainty of the CNT wall thickness leads to many theories and in turn paved for many results, ranged from about 1.0 to 5.5 Tpa of elastic modulus value. Chen and Liu [5] used square RVEs to derive material property based on elasticity theory. He used FEM method to study the load-carrying capabilities of the CNTs in a matrix and concluded with an improved value of elastic modulus of the composite matrix.

CHAPTER 3

OBJECTIVE AND MOTIVATION

3.1 OBJECTIVE

In this work, modeling of CNT involves the determination of Young's modulus that is responsible for some exceptional mechanical properties such as stiffness, tensile strength and resilience. This process of modeling first involves MD Simulation through LAMMPS and the resulting Young's modulus is validated with previous results of simulation work. The second phase of work involves FEM method through RVE (Representative Volume Element) technique that confirms the load carrying capacities of the CNTs in a matrix are significant because of the superior Young's modulus value.

3.2 MOTIVATION

Since the experimental study of CNT costs much because of its complexity at Nano- scale level that is very difficult in a direct experiment basis, so computer simulations are the one approach that is time-saving and economical. This simulation technique has one more advantage of making execution process for large-scale model faster than other methods. To use MD simulation in research work various software are available in present days that are like Abalone, Chemistry at Harvard Macromolecular Mechanics (CHARMM), Large Atomic/Molecular Parallel Simulator (LAMMPS) etc. Since current project work involves Nano- scale work, this LAMMPS software is very useful. MD simulation also has some limitations on the use of CNT in real world applications. It has an application constraint in terms of small length and time scales and not suitable for the larger length scales in studying nanocomposites. For engineering applications, nanocomposites must expand from nano to macro length scales. In addition to that, after obtaining the value of Young's modulus from simulation result finite element method (FEM) is used for deriving properties of CNT-based composite.

CHAPTER 4

METHODOLOGY

4.1 Atomic structure of CNT

The CNTs are of two types that are single-walled and multi-walled. Multi-walled carbon nanotubes (MWCNTs) were manufactured by co-axially placing single-walled carbon nanotubes (SWCNTs) of different radii. There are few ways to view SWCNT, and the most used is by rolling up graphene sheet to construct a hollow cylinder with end caps. The cylindrical wall is made of hexagonal carbon rings, and the end caps are of pentagonal rings. This unit cell that is a hexagonal ring is repeated sequentially by the virtue of covalent bonds with neighboring carbon atoms. The covalent bond between these carbon atoms is an exceptionally strong chemical bond that has an important role for exceptional mechanical properties of the graphite structure. The atomic structure of CNTs depends on the chirality of tube structure. This chirality is defined by two parameters that are chiral vector Ch and the chiral angle Θ. The chiral vector Ch is indicated by the lattice translational indices (n, m) and two basis vectors a1 and a2. The chiral angle Θ is represented as the angle between the chiral vector Ch with the zigzag direction of the graphene sheet.

$$C_h = n\vec{a1} + m\vec{a2}$$

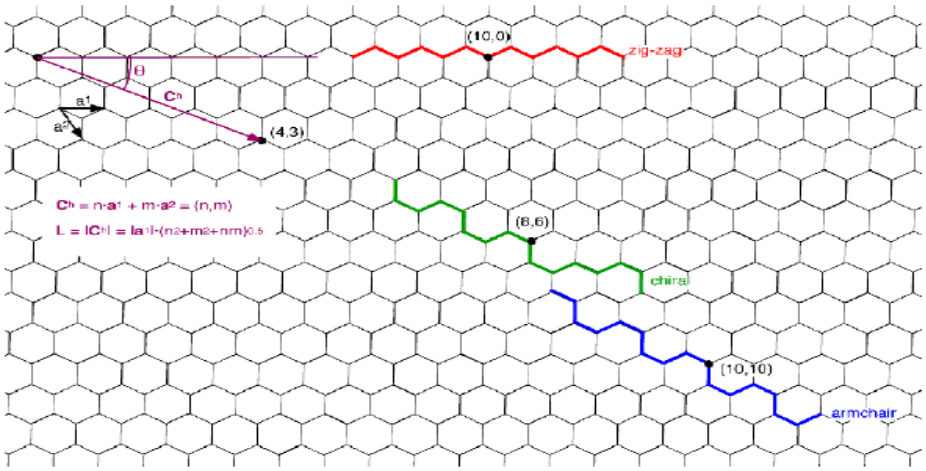
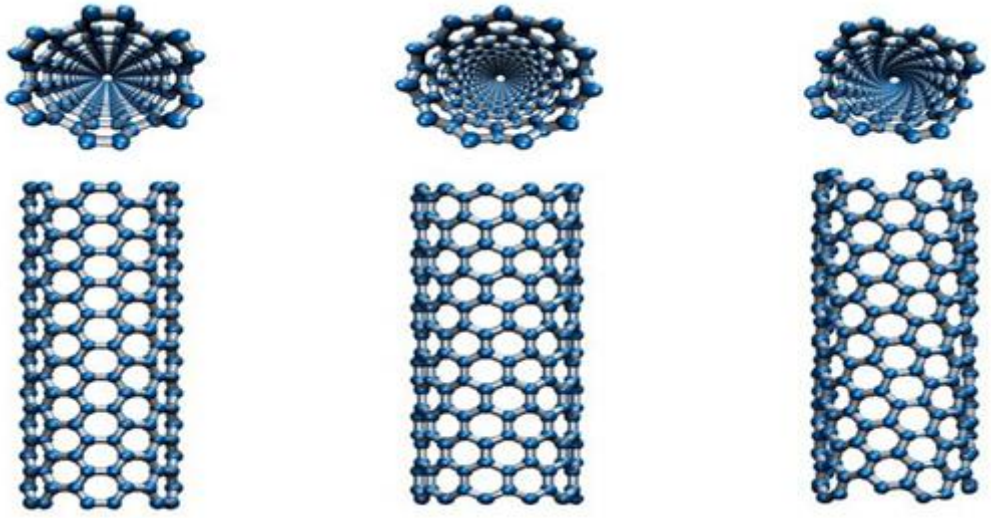


Figure 4.1 Graphene layer with carbon atoms labeled using (n, m) notations

Depending on the chiral angle and lattice translation indices carbon nanotubes are divided into three types:

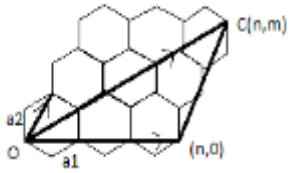
- Nanotubes with chiral angle 0 and translational indices such as (*n*, *n*),armchair structure is formed
- Nanotubes with chiral angle 30 and translational indices such as (*n*,*0*),zigzag structure is formed
- A nanotube with chiral angle from 0-30 and vector notation (*n*, *m*), $n \neq m$, chiral structure is formed.

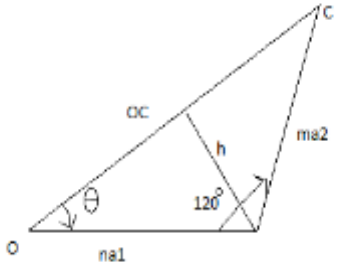


Armchair Zigzag Chiral

Figure 4.2 Front view and top view of the different types of carbon nanotubes

The physical properties of carbon nanotubes are determined by their diameter and chiral angle, both of which are function of *n* and *m*. Diameter and chiral angle can be calculated in terms of *m* and *n* as below:





$$OC = \sqrt{(na1)^2 + (ma2)^2 + 2(na1)(ma2)\cos 60}$$

$$= a\sqrt{n^2 + m^2 + 2nm \times 1/2}$$

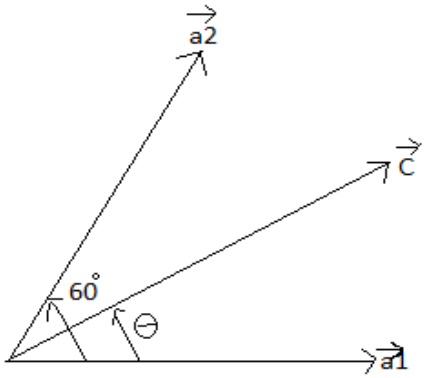
$$= a\sqrt{n^2 + m^2 + 2nm}$$

$$|\vec{a1}| = |\vec{a2}| = a = 0.246 \text{ nm}$$

Diameter of cnt $= \frac{perimeter}{\pi} = \frac{|\vec{C}|}{\pi}$

$$= \frac{0.246\sqrt{n^2+m^2+2nm}}{\pi} \text{ (nm)}$$

For chiral angle:



$$\cos\theta = \frac{\vec{c}\cdot\vec{a1}}{|\vec{c}|\,|\vec{a1}|} = \frac{\left(n\vec{a1}+m\vec{a2}\right)\cdot\vec{a1}}{a^2\sqrt{n^2+m^2+2nm}}$$

$$= \frac{na^2+ma^2\times\cos 60}{a^2\sqrt{n^2+m^2+2nm}}$$

$$= \frac{2n+m}{2\sqrt{n^2+m^2+2nm}}$$

$$\text{Sin}\,\theta = \sqrt{1-cos\theta^2}$$

$$= \sqrt{1-\frac{(2n+m)^2}{4(n^2+m^2+nm)}}$$

$$= \frac{\sqrt{3}\times m}{2\sqrt{n^2+m^2+nm}}$$

According to research, chiral vector (n, m) and chiral angle determines various different structures of CNT.

4.2 Modeling and Simulation of Carbon Nanotube

4.2.1 Simulation

A simulation is the technique of approximating the behavior of some system or situation by means of an equivalent model, situation, either to pick up data more promptly or to prepare personnel. A simulation is carrying out a model, presented by a computer program that gives information about the studied system. The simulation technique of analyzing a model is different to the analytical approach, where the method of analyzing the system is purely hypothetical. As this approach is more solid, the simulation practice gives more flexibility and comfort.

❖ **MD Simulation**

Molecular dynamics is a technique that allows an arithmetical "thought experiment" to be carried out using a model that, to a partial extent, estimates a real physical or chemical system. Such a "virtual laboratory" tactic has the benefit that many "experiments" can be easily set up and carried out in sequence by simply changing the control parameters. The obvious limitation is that the results are only as good as the statistical model. Add to that the results can be artificially

inclined if the molecular dynamics calculation is unable to sample a substantial number of microstates over the time it is allowed to run. MD is a computer simulation of physical movements of atoms and molecules. These atoms or molecules are permitted to work together for a particular time, which gives a perception of the movement of the particles. In this method, the paths of atoms and molecules are found by mathematically solving Newton's equations of motion. Here required forces and energy are defined by inter-atomic potentials or molecular mechanics force fields. A range of software used for MD simulation in modern day research work. But this particular project work uses LAMMPS (Large Atomic Molecular Massively Parallel Simulator) for simulation purpose.

- **LAMMPS**

LAMMPS is a conventional molecular dynamics code that models a collection of particles in all 3 probable states. This tool can be used to model different systems from various fields starting from polymeric to coarse-grained systems.

Basic inputs for simulation process

Execution of simulation involves some basic input and output files in which 2 basic input files are very much necessary to start a simulation process. These basic input files are commonly called 'in' file and 'potential file'.

LAMMPS 'in' file (input script)

This simulation is run by reading various commands from an input script which is a text file. LAMMPS executes these commands line by line and each command results in a certain action.

Input script Structure

The input script of LAMMPS includes four basic parts:-

1) Initialization
2) Atom definition
3) Settings
4) Running simulation

(1) Initialization

LAMMPS code is started with this part where various parameters are set before creating atoms for simulation process.

(2) Atom definition

There are 3 fundamental ways of defining atoms in LAMMPS. These are reading it from a data file or restart file with the help relevant commands (read_data, read_restart) or creating atoms on a lattice using certain commands.

(3) Settings

Once atoms and molecular topology are stated, a range of settings are supplied. These settings define various force fields and required potential for interaction between atoms or molecules.

(4) Running simulation

This part is the last section of LAMMPS coding where run command is used to run a MD simulation with required number of iterations.

LAMMPS Potential file

Generally in MD simulation as already mentioned a potential file is needed which defines a particular way of interaction. For different simulations which use MD method, there are different types of potential files. In general for LAMMPS, Embedded Atom Method (EAM) potential is used. E.g.:- Al_zhou.eam.alloy, co_Al.eam.alloy etc. Here developing model of CNT, Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential is used which defines the interaction between carbon atoms.

AIREBO Potential

The AIREBO pair style calculates the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential for a system of carbon, hydrogen atoms or combination of both.

The AIREBO Potential includes three terms:

$$E = \frac{1}{2}\sum_{i}\sum_{j\neq i}\left[E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k\neq i,j}\sum_{l\neq i,j,k} E_{kijl}^{TORSION}\right]$$

LAMMPS Output file

Output files basically are of four types:-

Thermodynamic output (log file)

Dump files (For visualizing the molecular structure)

User-specified files (With help of fix command certain quantities are stored in this file)

Restart files

Visual Molecular Dynamics (VMD)

VMD is developed as software for visualizing and analyzing results obtained through MD simulation. This software uses particular input file formats such as output files of LAMMPS and other MD simulation work.

Steps to be followed for simulation process

1) Developing the structure of carbon Nanotube:

This simulation work is based on a single walled armchair carbon nanotube with lattice translational indices (9, 9) and length 6.5 nm .

As stated before for atom definition part there are three way to define a particular structure. Here this is ensured by reading one topological data file (data file) created with the help of VMD nanotube builder.

For developing nanotube structure, some input data such as topology building data and nanotube building data are necessary.

Topology building data: Length of c-c bond in nanometer: 0.14418 nm

Nanotube building data: Nanotube chiral index n: 9

Nanotube chiral index m: 9

Nanotube length in Nanometer: 6.5nm

Resulting data file includes no. of bonds, angles, dihedrals, improper and the corresponding structure can be shown as below.

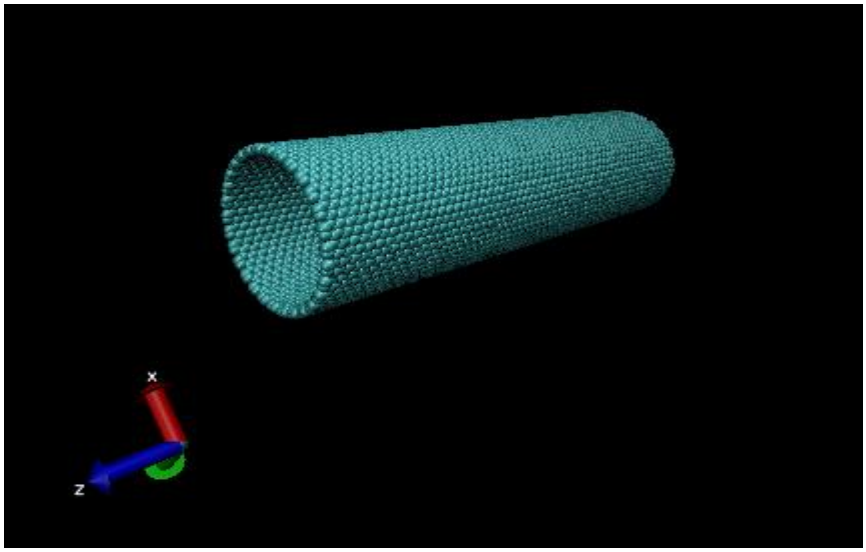


Figure 4.3 Armchair structure of CNT (9, 9) developed through VMD

2) Initialization and settings part for the coding are set through relevant commands. Force field is selected using pair_coeff command. Required airebo potential is used through pair_style command.

3) Relaxing the initial configuration to reach the equilibrium state: For this purpose 'fix npt' command is used and after 20000 runs again it is unfixed.

4) Final cell length is stored for strain calculations and boundary condition is fixed at one end of the tube through 'fix npt' command. Strain rate is set through 'fix deform' command so that corresponding stress and strain value can be calculated for 20000 iterations.

5) Stress and corresponding strain values are stored in cnt_stress_strain.txt file and thermodynamic output parameters are displayed for 20000 iterations.

6) These output stress and strain values are used for calculation of young's modulus of single-walled armchair carbon nanotube.

The above simulation provides an output file with stress and strain data which is important for the evaluation of young's modulus and presented in Table 1.

Table 4.1 Complete set of Output stress and strain data by MD simulation

Strain	Stress
0.006802	6.327882373
0.006809	6.335551557
0.006813	6.342572244
0.006819	6.349318191
0.006832	6.355763897
0.006837	6.362525873
0.006845	6.370299067
0.006856	6.380879267

4.2.2 FEM Modelling

In Engineering problems there are some basic unknowns. If they are known the behavior of entire structure can be predicted. The basic unknown or field variables which are encountered in engineering problem are displacement in solid mechanics velocity in fluid mechanics etc. In a continuum these elements of unknowns are infinite. The finite element method minimizes these unknown variables to finite numbers by dividing solution region into small portions called elements. The appropriate functions are defined in term of field variables of specified points called nodes/nodal point. Once these are found, the field variables at any point can be known by using interpolation functions.

.

Significance of Representative Volume Element (RVE)

This is an important theory for composite materials where representative volume element (RVE) is the smallest volume over which a measurement can be made that will produce a value representative of the entire volume. This method includes mechanical properties such as elastic moduli, hydro-geological properties, electromagnetic properties and other averaged quantities to explain physical systems.

Modeling of CNT based composite (matrix) using RVE

Carbon Nanotubes (CNTs) have the potential to provide suitable reinforcing materials for the growth of a new section of Nanocomposites. It is found that when 1% (by weight) of CNTs added to a matrix material, the stiffness value of the resulting composite film increases leading to a superior load-carrying capacity.

Methodology

Mechanical properties such as young's modulus and Poisson's ratio of CNTs have been successfully anticipated by using continuum approaches. The material property of the CNT-based composites deals with the overall mechanical responses of the RVEs. Thus, the continuum method is very much suitable for the present study, although further improvement and acceptance are needed.

Steps to be followed

STEP-1

A 3-D elasticity model is used here for modeling the CNT embedded in a matrix. This model ensures the correctness and compatibility of the model consisting of CNTs and matrix. Before proceeding further first, this model is to be generated using ANSYS Parametric Design Language (APDL).

STEP-2

This step is used as formulation of effective mechanical property i.e. Young's modulus of CNT-based composite using elastic theory.

STEP-3

CNT inside the matrix material is studied using the FEM in this part. This step includes deformation and stress analysis for axial loading of the CNT-based matrix so that Young's modulus can be calculated.

STEP-4

The results obtained are validated with analytical results based on Rule of Mixture (ROM). This method uses volume fraction of carbon nanotube in whole composite matrix element to evaluate the elastic modulus value.

Model Development

STEP-1

Here the model which is a Long CNT, through the length of a square RVE is modelled using ANSYS 15(APDL). Since it is a 3-D model quadratic solid (brick) element is used.

The dimensions of model: (For the matrix): length L= 100 nm, a =10 nm (half of width)

(For the CNT): length L =100 nm, outer radius r_o = 5 nm, inner radius

r_i = 4:6 nm (effective thickness = 0.4 nm)

The Young's moduli and Poisson's ratios used for the CNT and matrix are:

CNT: E_t = 1000 GPa; μ_t= 0:3;

Matrix: E_m= 100 GPa; μ_m = 0:3:

After creating this part then both matrix and CNT are combined by an operation called glue which confirms the load would be taken by both of them when axial load will be applied.

Next step is the meshing of the above part where fine mesh setting ensures the accuracy of model preparation. Then this part is extruded so that complete matrix containing the CNT can be prepared. The part after this operation is shown in Figure 4.4.

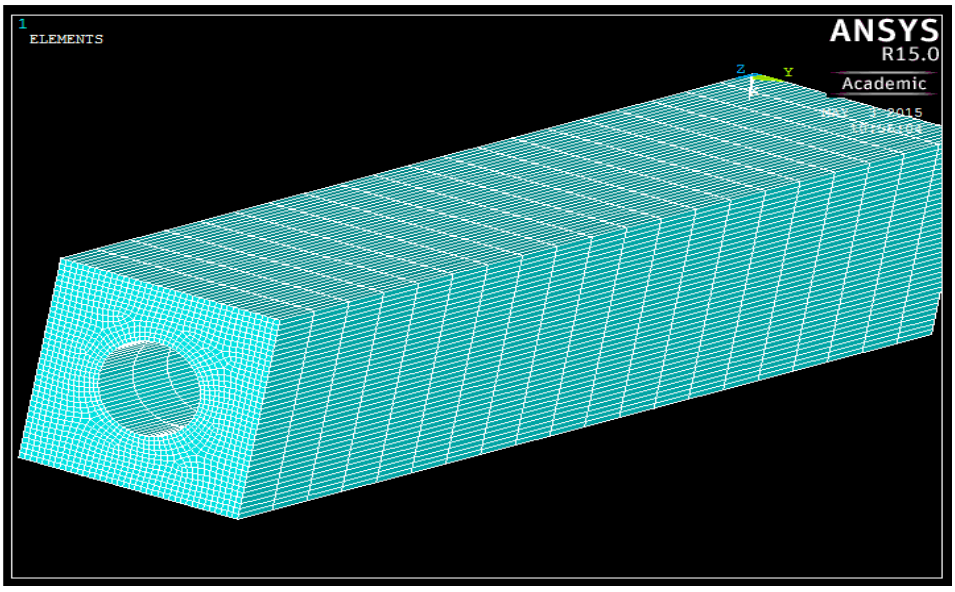


Figure 4.4 Finite element mesh of the square RVE extruded along z-direction

By setting degree of freedom (DOF) of one end is zero (fixing this end), displacement of 2 nm is provided so that whole part will be deformed and accordingly stress and strain will be developed.

STEP-2

The formula for the equivalent material constant a homogeneous and elastic model of square RVE is selected. The elastic model is packed with a transversely isotropic material. Among the four effective material constants, Young's modulus in axial direction i.e. E_z is needed to be calculated.

The general 3-D strain–stress relation connecting the normal stresses $(\sigma_x, \sigma_y, \sigma_z)$ and strains $(\varepsilon_x, \varepsilon_y, \varepsilon_z)$ can be written as:

$$\begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \end{Bmatrix} = \begin{bmatrix} \frac{1}{E_x} & -\frac{\nu_{xy}}{E_x} & -\frac{\nu_{zx}}{E_z} \\ -\frac{\nu_{xy}}{E_x} & \frac{1}{E_x} & -\frac{\nu_{zx}}{E_z} \\ -\frac{\nu_{zx}}{E_z} & -\frac{\nu_{zx}}{E_z} & \frac{1}{E_z} \end{bmatrix} \begin{Bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{Bmatrix}$$

To derive expression for E_z value, axial loading condition is established which is shown below:

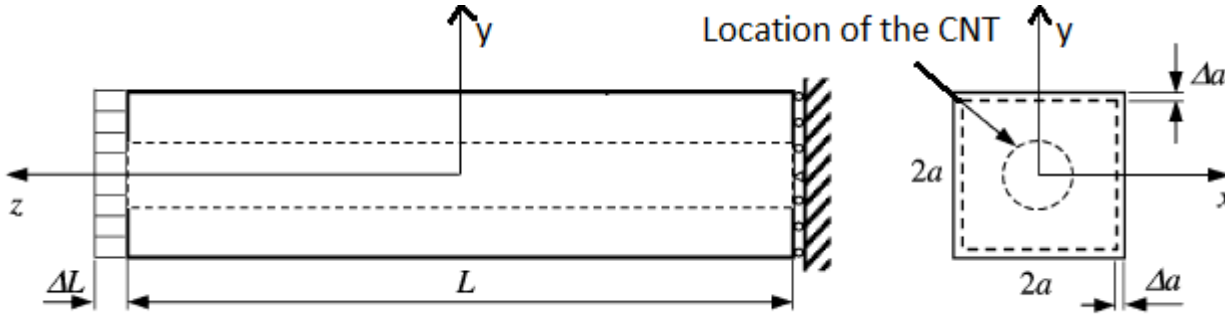


Figure 4.5 Square RVE Under axial stretch ΔL to evaluate the effective material properties

Square RVE applied with an axial stretch ΔL:

In this case (Figure 4.5), the stress and strain components on the lateral surface are:

$$\sigma_x = \sigma_y = 0, \quad \varepsilon_z = \frac{\Delta L}{L}, \quad \varepsilon_x = \frac{\Delta a}{a} \text{ along}$$
$$x = \pm a, \quad \text{and} \quad \varepsilon_y = \frac{\Delta a}{a} \text{ along } y = \pm a,$$

Where, Δa is the change of dimension '*a*', under the stretch ΔL in the z-direction.

$$E_z = \frac{\sigma_{\text{ave}}}{\varepsilon_z} = \frac{L}{\Delta L}\sigma_{\text{ave}},$$

Where, the average value of stress σ_{ave} is given by:

$$\sigma_{\text{ave}} = \frac{1}{A}\int_A \sigma_z(x, y, L/2)\,\mathrm{d}x\,\mathrm{d}y,$$

'*A*' is the area of the end surface. The value of σ_{ave} is evaluated for the RVE using the FEM results.

CHAPTER 5

RESULTS AND DISCUSSIONS

5.1 SIMULATION RESULT

The output simulation data for armchair structure of (9, 9) nanotube comes out to be as following.

Table 5.1 Output stress and strain data from simulation process

Strain	Stress
0.006802	6.327882373
0.006809	6.335551557
0.006813	6.342572244
0.006819	6.349318191
0.006832	6.355763897
0.006837	6.362525873
0.006845	6.370299067
0.006856	6.380879267

For the calculation of Young's modulus value stress and strain values for certain number of iterations is taken where values not coming in the elastic range are discarded.

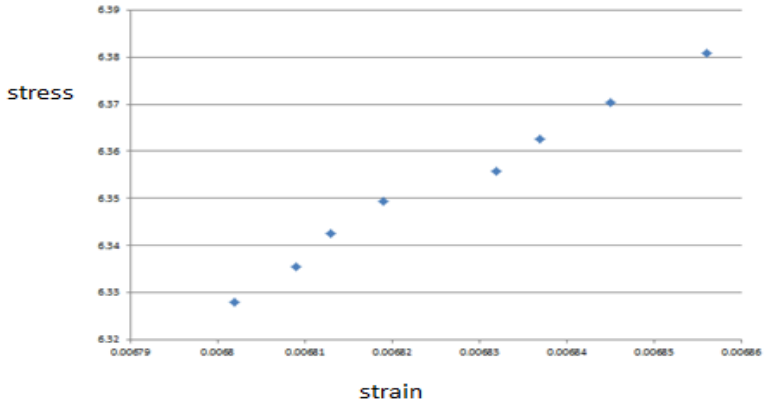


Figure 5.1 Stress-Strain graph for (9, 9) armchair SWCNT

The value of Young's modulus is obtained as 930.53 TPa from the Figure 5.1. This is the tensile modulus of carbon nanotube which shows far superior property for modern day composites application. For creating different nanotubes and their topological data file, VMD nanotube builder is used where (n, m) and length of tube are two inputs required for developing the same.

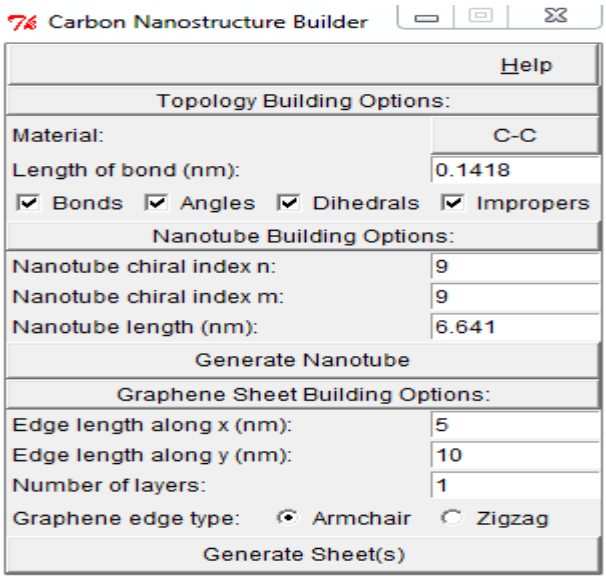


Figure 5.2 Carbon Nanostructure Builder Input Parameters

Now by changing the chiral index of carbon nanotubes a series of armchair structures are developed (using VMD Nanotube Builder) whose geometrical properties are listed in Table 5.2.

Table 5.2 Geometrical properties of different Nanotubes created in VMD Nanotube builder

(n, n)	No. of atoms	Radius	Length (nm)
(6, 6)	456	0.407	4.427
(7, 7)	616	0.475	5.165
(8, 8)	800	0.543	5.903
(9, 9)	1008	0.611	6.501
(10, 10)	1240	0.678	7.379
(11, 11)	1496	0.746	8.116
(12, 12)	1776	0.814	8.554

Now, corresponding to the data from Table 5.2, nanotubes data files are created and used in the coding to determine Young's modulus in the same process like (9, 9) nanotube. The resulting young's modulus values obtained are tabulated in Table 5.3, and the average Young's modulus value is obtained as 0.9298±0.0009 Tpa. These obtained results in Table 5.3 can be validated using previous MD simulation work and presented in Table 5.4.

Table 5.3 Elastic moduli of single-walled carbon nanotubes

(n, n)	Young's modulus(E) (TPa)
(6, 6)	0.9289
(7, 7)	0.9304
(8, 8)	0.9301
(9, 9)	0.9305
(10, 10)	0.9308
(11, 11)	0.9308
(12, 12)	0.9306

Table 5.4 Comparison of MD and VMD of single-walled carbon nanotubes

Tensile Modulus	Wernik [11]	Shokrieh [12]	Lu [10]	Present Work
(Tpa)	0.9448	1.033-1.042	1.067-1.197	0.929 - 0.931

5.2 RVE ANALYSIS AND RESULT

After model development and formulation part in the methodology section, the deformed matrix element is analyzed through both deformation and stress analysis. Resulting stress and strain variation along the matrix element in z-direction is presented in Figure 5.3 and Figure 5.4, respectively.

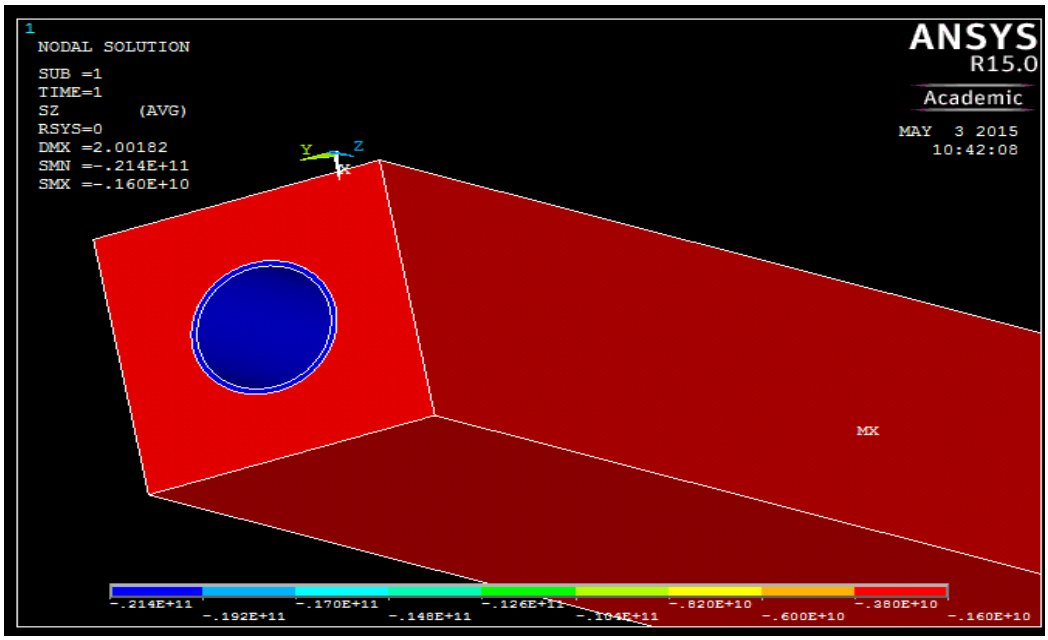


Figure 5.3 Stress variation along the length of matrix element

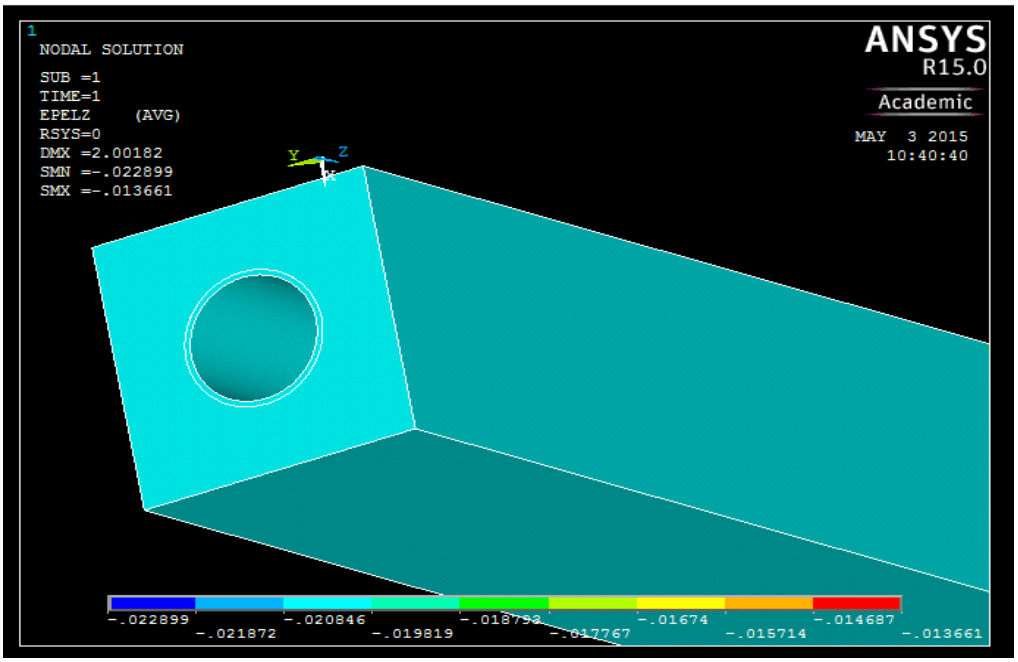


Figure 5.4: Variation of strain along the length of matrix element

Due to the axial load at the fixed end, a reaction force will act along z-direction, and this force is varied with the length. Average of this force value is used to calculate average stress i.e. σ_{ave}. Reaction force variation along the node is presented in Table 5.

Table 5.5 Reaction force variation along matrix element

NODE	Reaction force(FZ)
1	0.20505E+10
2	0.20549E+10
3	0.20685E+10
4	0.20449E+10
5	0.17987E+10
6	0.17987E+10
7	0.17987E+10
8	0.17987E+10
9	0.20474E+10
10	0.18709E+10

Based on the Table 5.5 the average Reaction force is obtained as 0.1933319E+10 and based on that the average stress is σ_{ave} = 5.0342 GPa. From strain analysis the average strain is calculated as (0.342)/10 = 0.0342

Hence, the Young's modulus is $E_z = \frac{\sigma_{ave}}{\varepsilon_z}$ = (5.0342)/ 0.0342 = 147.2 GPa.

Calculation of Elastic Modulus through Rule of Mixture (ROM)

As stated in step-4 of methodology section this result must be validated using Rule of mixture. This model use CNT through the length of the RVE for which volume fraction is to be calculated. For the square RVE, the volume fraction of the CNT is defined by-

$$V^t = \frac{\pi(r_o^2 - r_i^2)}{4a^2 - \pi r_i^2} = \frac{\pi(25-4.6^2)}{(4\times10^2-\pi\times4.6^2)} = 0.03617$$

Effective Young's modulus E_z in the axial direction is given as:

$$E_z = E^t V^t + E^m(1 - V^t) = 1000\times 0.03617 + 100 \times (1 - 0.03617) = 132.553$$ GPa

Where, E_t is the Young's modulus of the CNT and E_m is Young's modulus of the matrix.

From above result E_z / E_m = 1.325 (As E_m = 100 GPa).

Both these results obtained through RVE and ROM can be validated by comparing result obtained before in same field of work and presented in Table 5.6.

Table 5.6 Modulus ratio of square RVE by X.L. Chen &Y.J. Liu using FEM and ROM

FEM Model	E_z/E_m		E_z/E_m	
	FEM[5]	ROM[5]	ROM [Present]	ROM [Present]
3-D, single CNT	1.3255	1.3255	1.472	1.325

CHAPTER 6

CLOSURE

6.1 CONCLUSIONS

In this present work the material property is obtained by using MD simulation and in the later part this CNT is used in the composite matrix to obtain a higher Young's modulus value of the CNT embedded matrix. The present model is validated with the available published literature, and it is observed that the present results are in the expected line. In the present work, AIREBO potential is used for obtaining the value of Young's modulus, and it is found that the small amount of difference is there, and the reason behind this is different potential. Based on the Young's modulus results obtained through simulation process, the FEM modelling is used to confirm the application of CNT in the composite world through RVE technique and validated through Rule of Mixture (ROM).

6.2 FUTURE SCOPE OF THE WORK

For the simplification purpose, the CNT is taken as without any cap, but ideally speaking the cap that surrounds the both ends of the tube should be considered. Since this modeling process through MD simulation process involved only single walled carbon Nanotube, this work can also be extended for multi-walled carbon nanotube (MWCNT) which has some advantage over SWCNT in terms of mechanical and other physical properties. RVE technique using FEM method used a square RVE of a matrix element in the second phase of work. But these representative volume elements can be of different shapes like cylindrical and hexagonal. So, this work can be extended using these two types of representative volumes.

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