Prediction of Thickness Influence on the Mechanical Properties of Carbon Nanotubes using FEM

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Abstract: **An analytical molecular structural mechanics model for the prediction of mechanical properties of defect free and defected carbon nanotubes is developed by using finite element method. The finite element models are developed using FE software Ansys. The developed models are capable of predicting Young's moduli, Poisson's ratio of carbon nanotubes under cantilever loading conditions. The response of finite element models showed that the mechanical properties of single walled carbon nanotubes Young's moduli are sensitive to the tube thickness. Young's modulus and Poisson's ratio of armchair (3, 3) carbon nanotube with defect free, vacancy defect and stone wales defect is determined and the results are verified with existed literature for defect free condition.**

Keywords: **Carbon Nanotubes, Molecular Modeling, stone wales, Vacancy defect, Finite element method.**

I. INTRODUCTION

Carbon nanotubes [1], since their discovery in 1991, have attracted much interest due to their ability ofsustaining large deformations, their elevated stiffness and possible high strength. When two dimensions are in the nanometer scale and the third is larger, forming an elongated structure, they are generally referred as nanotubes. Carbon nanotubes are cylinders of graphene with diameters from 1 to 2 nm. They have single or multiple layers of carbon atoms in the tube thickness direction, and are called Single-wall Carbon Nanotubes (SWCNTs) and Multi-wall Carbon Nanotubes(MWCNTs) respectively. Due to the application of carbon nanotubes (CNTs) in Nano composites, investigation of elastic modulus will be very useful. Briefly the application of carbon nanotubesin several fields is shown by Fig.1 the Nano tubes can be used to prepare composites, coatings and adhesives. Even CNTs find theirapplication in medical and electrical and electronics domain [2].

Elastic responses of single as well as multi walled carbon nanotubes have been explored widely through theoretical and experimentation approaches. For an example, Mohammad pour et al. [3] predicted Young's modulus and poisons ratio calculated by finite element based software Ansys. Feng Dai-Li et al [4] focused their research on the stone-wales and vacancy defects influence on the thermal conductivity of CNTs using molecular modeling. Antonio F et al. [5] evaluated the response of CNTs using molecular methodology. Multi stone wales effect and vacancy defects influence on the mechanical behavior of carbon nanotubes are identified with molecular dynamics by Kamal Sharma et al.

As the application of CNTs are raising continuously, the knowledge over the mechanical properties are needed for their better design.

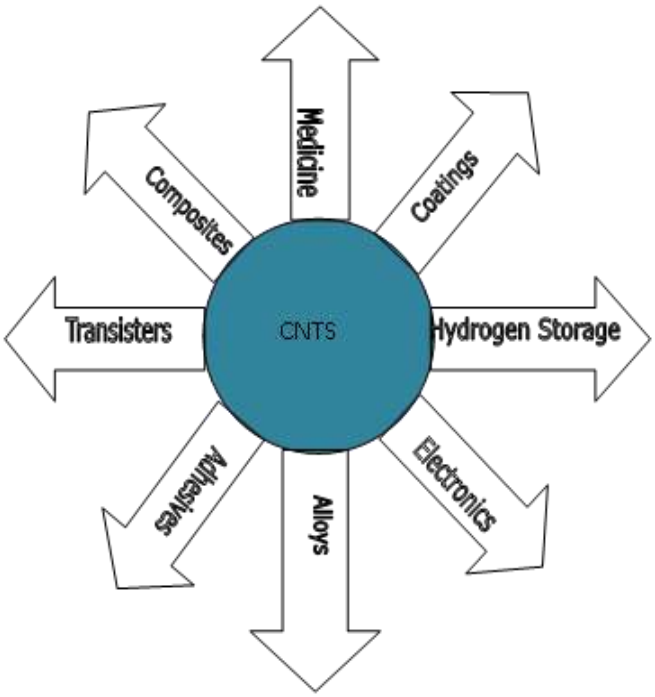

Fig. 1 Applications of carbon nanotubes

[6]. A structural based mechanics approach is applied to the CNTs by Li c at al [7]. A finite element modeling of CNT is developed by Tserpes KI and Cheng-Wen Fan [8 and 9] to disclose the mechanical properties of CNTs. Improved molecular structural mechanics approach is devoted to extract the Poisson's ratio of graphene and single walled carbon nanotubes by P. Zhao et al., [10]. From the above mentioned literature, the methodology to deal the carbon nanotubes with molecular mechanics approach is identified. Theobjective of the present work is to identify the influence thickness on Young's modulus and Poisson's ratio of carbon nanotubes with theapplication of molecular modeling approach. The predictions includethe defect free and defected nanotube characterization with respect to the thickness.

II. PROBLEM MODELING

The CNTs are obtained by rolling the graphene sheet. The way the sheet rolled generated arm chair, Zigzag and chiral tubes. Firstly, the graphene sheet is modeled in Pro-e software by considering length of the carbon bond as 0.34nm. Later these tubes are imported in finite element software Ansys.

2.1 Finite Element Modeling

The three dimensional armchair (3, 3) type carbon nanotube model is drawn with the use of PRO-Engineer Wildfire (version 2.0) software. Then these models are imported into ANSYS software through IGES file. The imported 3D models are recreated using the ANSYS commercial FE model. To create the FE models, nodes are placed at the locations of carbon atoms and the covalent bonds between them are modeled using three-dimensional elastic BEAM4 ANSYS elements.

A BEAM4 ANSYS element is a uni-axialelement with have the capabilities of tension, compression, bending and torsion. The element has six degree of freedom at each node: translations in the nodal x, y, and z directions and rotation about the nodal x, y, and z axes. The element is defined by two or three nodes, the cross-sectional area, two area moments of inertia (IZZ and IYY) and material properties. The cross sections of the beam elements are assumed to be uniform and circular, and the necessary input data of the BEAM4 elements are the Young`s modulus (E), the Poisson's ratio (ν) and thediameter of the circular cross section element is $d$. To calculate the Young`s modulus of the elements, a linkage between molecular and continuum mechanics is used which was proposed by the Li and Chou [11].That is, a linkage between the force fields constants in molecular mechanics and the element stiffness parameters in structuralmechanics through the energy equivalence concept. From theviewpoint of molecular mechanics, CNTs may beregarded asmolecules consisting of carbon atoms. The elastic modulus (E) can be determined by equating the energies due to the inter-atomic interactions and the energies due to deformation of the structural elements of the space frame.

Molecular mechanics = Structural mechanics

$$Kr = \frac{EA}{L}\ ,\ K\Theta = \frac{EI}{L}\ ,\ K\tau = \frac{GJ}{L},$$

Kr, $K\Theta$,$K\tau$are the force constants, there values are $6.52 \times 10^{-7}\ Nnm/rad$, $8.76 \times 10^{10}\ Nnm/rad$, $2.78 \times 10^{-10} Nnm/radand\frac{EA}{L},\frac{EI}{L},\frac{GJ}{L}$ are the element stiffness. We know that diameter i.e. thickness of single wall carbon nanotube is 0.34nm and elastic modulus

$$E=\frac{\sigma}{\varepsilon} = \frac{P/\pi t D_O}{\Delta L/L_O} = \frac{PL_O}{\pi t \Delta L D_O} \qquad \text{eq (1)}$$

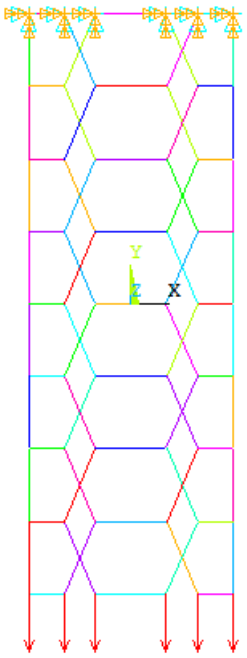

Fig.2 Fe model of (3, 3) arm chair without ant defect.

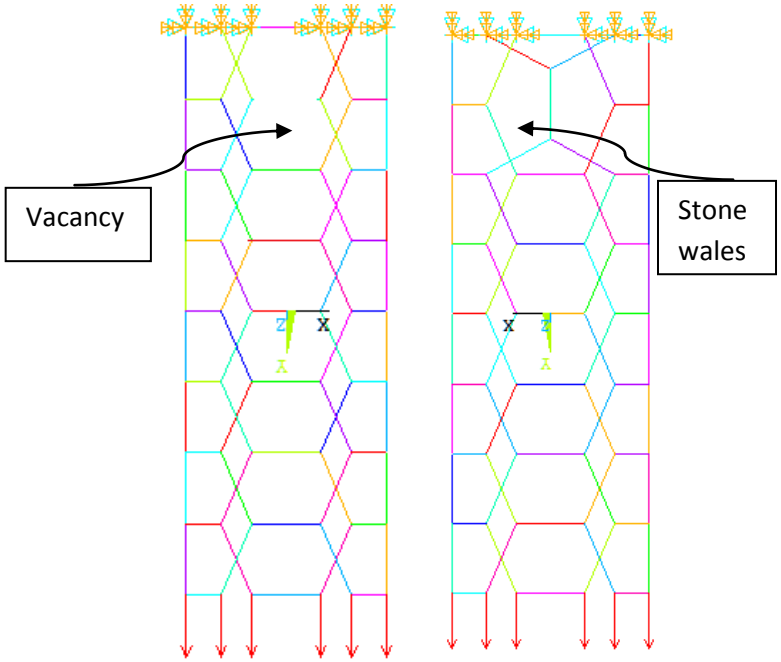

Fig.3 Fe model of (3, 3) arm chair with Vacancy defect and stone wales defect.

2.2 Validation

The finite element model is validated by comparing the Young's modulus of the carbon nanotube with existing literature.

The following table shows the Comparison of Young's modulus with published data.

TABLE 1

Investigator	Wall thickness (t)	Young's modulus E (TPa)	Present Fe model E (TPa) Value
Zang et al [12]	0.34	1.49	1.104
Treacy et al [13]	0.34	1.5	
A.Krishnan [14]	0.34	1.25	
Lu[15]	0.34	0.974	
Cheng Wen Fan [16]	0.34	1.0042	

III. RESULTS AND DISCUSSION

After the validation of the present FE model, the Young's modulus of the CNTs are estimated with defect free and vacancy defected and stone wales defected carbon nanotubes. As shown in Fig. 2 the prescribed forces are applied at oneend ofthe tube and the other end is fixed in all aspects. using equation (1) the Young's modulus ispredicted.Identifying laterral and longitudinal strains, the poisson's ratio is calculated. The Fig.4 shows the Young's moduli of arm chair (3,3) tube with differenent thicknesss by using Equation (1) from finite element models. It can be seen that the Young's modulus is decerses with the increasing the thickness of the CNT. The poisson's ratio is not reacted with the changes over the thickness in Fig.5 i.e it is almost constant with respect to the thickness of the CNT.

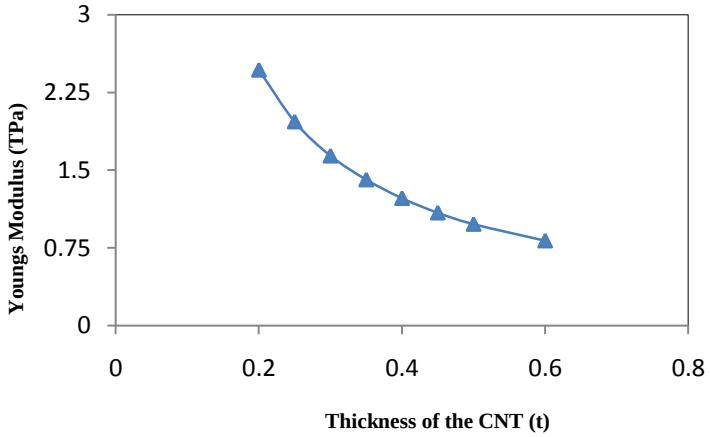

Fig.4Variation of Young's modulus with respect to thickness of arm chair CNT (3, 3)

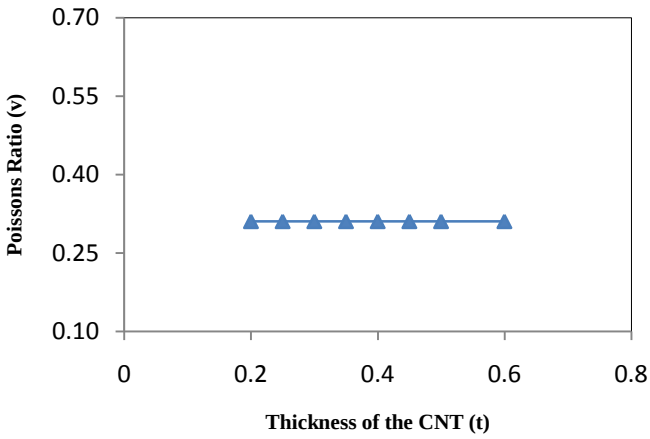

Fig.5Variation of Poisson's ratio withrespect to thickness of arm chair CNT (3, 3)

3.1 Influence of thickness on vacancy defected carbon nanotube

The defect free CNTs are existed in the ideal situation. However, the CNTs with vacancy and stone wales defects are frequently subjected defects in CNTs.Vacancy is nothing

but missing of carbon bond between atoms. The CNTs with vacancy defect is further decreased Young's modulus with rise in the thickness in Fig.6Still the Poisson's ratio is not responded with increasing the thickness even with vacancy defect as observed in Fig.7But the magnitude of Poisson's ratio is increased compared with defect free Poisson's ratio due to increase in the longitudinal elongation with defect.

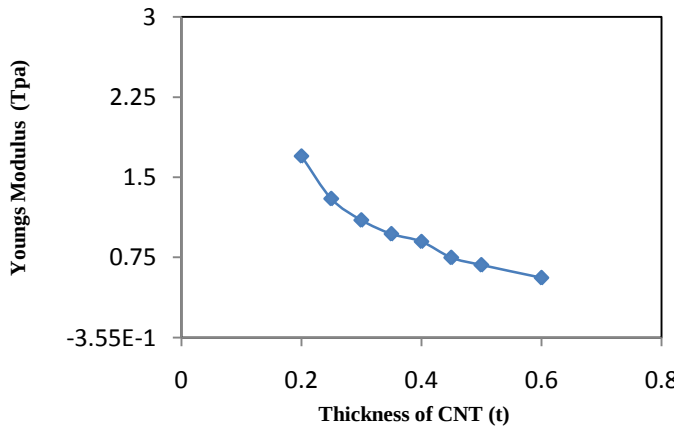

Fig.6 Variation of Young's modulus with respectto thickness of Vacancy defect arm chair CNT (3, 3)

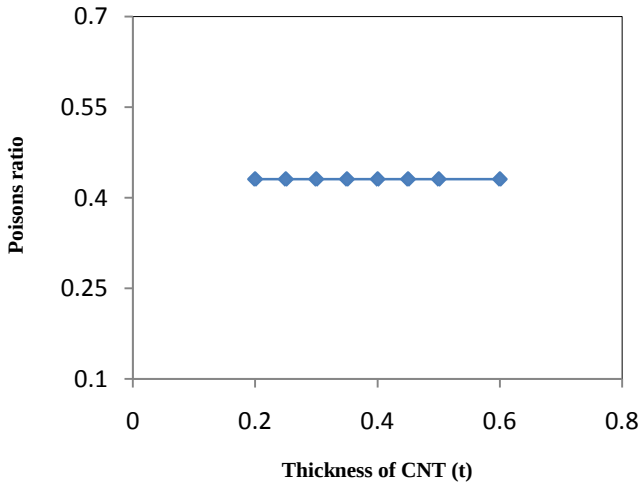

Fig.7Variation ofPoisson's ratio with respect to thickness of Vacancy defect arm chair CNT (3, 3)

3.2Influence of thickness on Stone wales defected carbon nanotube

Stone wales defect is generated by the rotation of two atoms by 90^0 with respect to midpoint as shown in the Fig.3the 5-7 stone wales defect is considered for the analysis. 5-7 stone wales means by the rotation of the carbon bond to 90^0 a pentagon adjacent to a heptagon neatly replaces two hexagons. The stone wales defect is adversely affected the Young's modulus than vacancy defects. The Poisson's ration of CNT is increased then compared to Poisson's ratio of vacancy defected CNT.

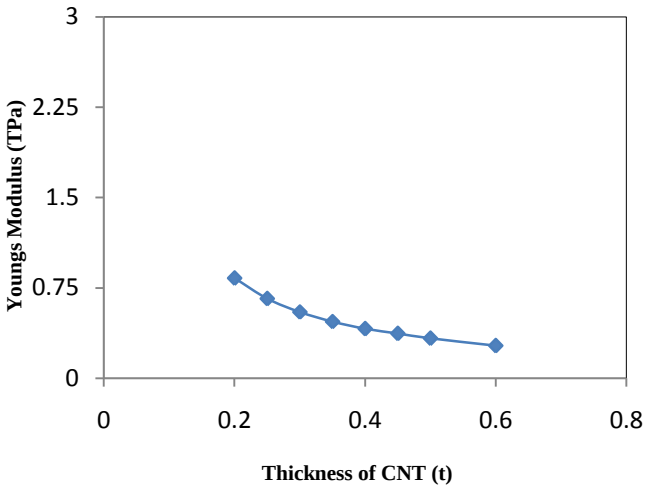

Fig.8 Variation of Young's modulus with respect to thickness of Stone Wales defect arm chair CNT (3, 3)

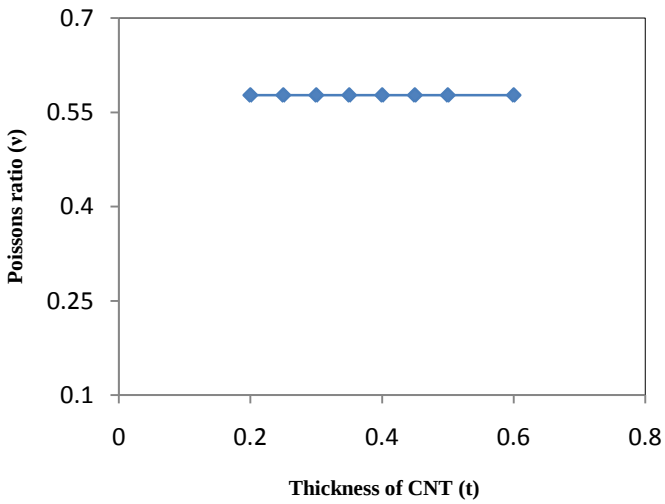

Fig.9 Variation of Poisson's ratio with respect to thickness of Stone Wales defect arm chair CNT (3, 3)

IV.CONCLUSIONS

By incorporating the finite element method into an analytical molecular structural mechanics, the mechanical properties of armchair nanotubes with vacancy and stonewales defect and defect free nanotube are investigated. The presentapproach is capable of predicting Young s moduli, Poisson's ratios of nanotubes. Young s moduli and Poisson ratios of nanotubes have been found to besensitive to their thickness. Generally arm chair nanotubes with stone wales defect reduced the Young's modulus than armchairnanotubes when they are experienced to vacancy defect. However, their Poisson's ratio is unchanged to their thickness and shows the same trends for both defects.

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