INVESTIGATION OF THE MECHANICAL PROPERTIES OF CARBON NANOTUBES, UNDER THE INFLUENCE OF IMPERFECTIONS

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“Nothing exists except atoms and empty space”

This thesis is dedicated to all people who endeavor to develop knowledge, and to my beloved and kind parents who always supported me and filled my heart with nothing but their love and finally to all peaceful people of Iran.

This dissertation is dedicated to my family especially my lovely parents, Ibrahim and Parvin and my dear brother, Mostafa for the support they provided me through my entire life.

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ABSTRACT

A carbon nanotube is a hollow cylinder, which is made of carbon atoms in the hexagonal lattice, which is made by rolling up the grahene sheet in the specific chiral vector direction. This cylindrical structure has outstanding mechanical, electrical thermal properties. Several attempts have been done to obtain the mechanical properties of CNTs in terms of Young's modulus, shear modulus, tensile strength etc. The finite element method has been used to obtain the Young's modulus of variety SWCNTs in this study. Furthermore, the imperfection (carbon vacancy) in the structure of SWCNT has been investigated on these models. Imperfection is one of the issues occurred in the producing of carbon structures such as graphene and carbon nanotubes and has a huge influence on mechanical properties of CNTs. This study consists of 68 different carbon nanotube models in three different types that are zigzag models from (3, 0) to (17, 0), armchairs from (2, 2) to (10, 10) and chiral models between (2, 2) and (10, 10). The imperfection percentages that investigated in this study are 5%, 10% and 15%. The results show that all models lose 34%, 56% and 90% of their tensile strength when they lost 5%, 10% and 15% of their carbon atoms from their structures (imperfection).

ABSTRAK

Satu tiub nano karbon adalah silinder berongga yang diperbuat daripada atom karbon dalam kekisi heksagon, yang dibuat oleh menggulung lembaran graphene dalam arah vektor kiral tertentu. Struktur silinder mempunyai mekanikal, sifat elektrik yang cemerlang terma. Beberapa percubaan telah dilakukan untuk mendapatkan sifat-sifat mekanik CNTs dari segi modulus Young , modulus ricih , kekuatan tegangan dan lain-lain Kaedah unsur terhingga telah digunakan untuk mendapatkan modulus Young pelbagai SWCNTs dalam kajian ini. Tambahan pula, ketidaksempurnaan itu (karbon kekosongan) dalam struktur SWCNT telah disiasat pada model ini. Ketidaksempurnaan adalah salah satu daripada isu-isu yang berlaku dalam operasi penghasilan struktur karbon seperti graphene dan nanotube karbon dan mempunyai pengaruh yang besar ke atas sifat mekanik CNTs . Kajian ini terdiri daripada 68 berbeza model tiub nano karbon dalam tiga jenis yang berbeza yang model mabuk dari (3, 0) kepada (17, 0) , kerusi-kerusi dari (2, 2) hingga (10 , 10) dan model kiral antara (2, 2) dan (10, 10). Peratusan ketidaksempurnaan yang disiasat dalam kajian ini adalah 5%, 10% dan 15%. Keputusan menunjukkan bahawa semua model kehilangan 34% , 56% dan 90% daripada kekuatan tegangan mereka apabila mereka hilang 5%, 10% dan 15% daripada atom karbon mereka dari struktur mereka (ketidaksempurnaan).

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LIST OF ABBREVIATION

C	-	Carbon
CNT	-	Carbon Nanotube
SWCNT	-	Single-Wall Carbon Nanotube
MWCNT	-	Multi-Wall Carbon Nanotube
FEM	-	Finite Element Method
MD	-	Molecular Dynamic
CM	-	Continuum Mechanic
AFM	-	Atomic Force Microscope
TEM	-	Transmission Electron Microscope
A	-	Cross-section Area
L	-	Length of CNT
t	-	Thickness of CNT
b	-	C-C bond length
D	-	Diameter of CNT

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CHAPTER 1

INTRODUCTION

1.1 Overview

From the ancient, humans were looking for strong materials in order to apply them in their daily uses, wars and simply to be alive. Since that time people found iron and its carbon alloys are the strongest materials in the world. After improving the sciences and finding the importance of the atoms and interaction between them, scientists found the atomic structures made by pure carbon may have the strongest structures. The famous pure carbon structure is diamond which being considered as a strongest structure for long time.

After first observation of carbon nanotubes (CNT) by Iijima in 1991 [11], all efforts have been concentrated on deriving the finite element model (FEM) in order to investigate the properties of CNTs, such as Young's modulus, shear modulus and etc. Nowadays, it has been observed that 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 bonds formed between the individual carbon atoms. Carbon nanotubes have outstanding Young's modulus, which is more than five times larger than stainless steel.

Beside the experimental investigations, many efforts have been done in order to investigate the mechanical properties of CNTs. Experimental and computational simulation such as molecular dynamics (MD) and continuum mechanics are the most important and useful methods in order to evaluate the characteristics of CNTs. The most powerful methods considered recently are computational methods due to the high costs involved in experimental to investigate the properties of CNTs. And the most commonly continuum mechanics technique is the finite element method (FEM), which is the computational approach to study the behaviors of CNTs. Based on these methods, different ranges of Young's modulus have been reported due to different length, different thickness or different computational or experimental approaches used to study the mechanical properties of CNTs. But, in most of them, the Young's modulus reported equal to 1 TPa approximately.

Li et al. [7] calculated the Young's modulus with respect to different nanotube diameters. They also, reported the Young's modulus ranges of CNTs are between 0.89 to 1.033 TPa. Changa et al. [5] represent the first effort to establish analytical methods of molecular mechanics and a set of examples that can be solved in closed form. They obtained that the Young's modulus is between 0.59 and 1.06 TPa. They reported for a given tube diameter, Young's modulus for armchair tubes is slightly larger than that for zigzag tubes.

Natsuki et al. [19] evaluated the Young's modulus ranges from about 0.5 TPa to more than 1.1 TPa depending on the wall thickness and the structure, whilst, Yu et al. [43] presented results of 15 SWCNT bundles under tensile load and found Young's modulus values in the range from 0.32 to 1.47 TPa. Krishnan et al. [42] of SWCNTs found an average modulus of about 1.3 $\pm$ 0.4 TPa for 27 SWCNTs.

1.2 Problem Background

Producing nano-materials or nano-structures due to non-precise facilities cause to have some problems in the perfect structure of CNTs. These problems are varying from doping other atoms, imperfection and perturbation of single carbon atoms and having all problems simultaneously in the structure of CNTs. However, because of lacking on experimental facilities in order to investigate the mechanical properties of CNTs specially disordered structures, the investigation based on computational methods such as continuum mechanics and FEM models have been considered recently.

1.3 Problem Statement

Since the first observation of single wall carbon nanotubes (SWCNTs) there have not been done any investigation on imperfect CNTs in all range of models. Finding a good description for imperfection models will be useful in order to know the effect of using these kinds of CNTs in composite materials. This study will answer to the question, what will happen to the Young's modulus of CNT if the structure will be affected by missing one or more carbon atoms and their related elements.

1.4 Aim of the Project

The goal of this project is to investigate the Young's modulus of imperfect CNTs and derive the best description of mechanical properties based on the imperfection percentage.

1.5 Objective of the Project

The objective of this project is to determine the Young's modulus as a property of different degrees of SWCNT under influence of imperfections.

1.6 Scope of the Project

The study is limited to the following scopes:

i. Literature review on carbon nanotubes and imperfections.
ii. Derive the finite element models for different SWCNT from Nanotube modeler.
iii. MATLAB will be used to code the imperfection in the CNT structures.
iv. The Finite element model of perfect and imperfect structure of CNTs will be evaluated in the MSC.Marc Mentat in order to investigate the Young's modulus.
v. The comparison between perfect and imperfect structures will get the better description on the effects of imperfection on the CNTs.

1.7 Organization of the Project

This report covers six chapters, which are introduction, literature review and research methodology, derivation of Young's modulus of perfect structures based on literature reviews, obtaining the Young's modulus of imperfect structures based on the imperfection percentages, comparison of findings and discussion about the results. Chapter one includes the introduction of the study, the problem statement, aim of the study, the objective, scope of the study, general methodology. Chapter two provides background information and a review of related literatures that leads to the problem statement. Chapter three provides the methodology of the study. In chapter four, the derivation of Young's modulus of perfect structures will be investigated and in chapter five, the Young's modulus of imperfect structures and the results will be discussed. The Young's modulus comparison between perfect and imperfect CNTs will be illustrated in chapter six and future work will be represented.

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