NUMERICAL SIMULATION OF COMPOSITE MATERIALS REINFORCED WITH CARBON NANOTUBES

RESAM MAKVANDI

A thesis submitted in fulfilment of the
requirements for the award of the degree of
Master of Engineering (Mechanical Engineering)

Faculty of Mechanical Engineering
Universiti Teknologi Malaysia

JUNE 2013

To my parents for their enormous financial and emotional support throughout my study.

ACKNOWLEDGEMENT

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

Besides, I would also like to thank my parents and two elder brothers. They were always supporting me and encouraging me with their best wishes.

Finally, I would like to thank my dear friend Mr. Siamak Fereidooni for all his support and encouragement throughout my study in Malaysia.

ABSTRACT

The application of carbon nanotubes (CNTs) in innumerable areas of industry is increasing day-to-day. One of their most important applications is in composite materials as the reinforcing phase. Many researchers studied the behavior of composite materials reinforced with short fibers. This paper examines the effect of the position of short fibers on the total stiffness of a composite material reinforced with carbon nanotubes for various volume fractions. Three different situations have been suggested for the position of a CNT fiber with respect to the other fibers in the composite: completely separated fibers, fibers with overlap, and fibers connected through a shared node (long fibers). Three different cases including a case when just overlaps are allowed, a case when just long fibers are allowed and a case when both overlaps and long fibers are allowed have been investigated. It has been shown that the effect of these cases on the Young's modulus of the composite is significant and that they should be considered for a better understanding of the reinforced composites behavior. In addition, it is shown that the effect of the investigated cases is more remarkable at higher numbers of randomness values.

ABSTRAK

Penggunaan nanotube karbon (CNTs) di kawasan begitu banyak industri semakin meningkat dari hari ke hari. Salah satu aplikasi yang paling penting mereka adalah dalam bahan komposit sebagai fasa memperkukuh. Ramai penyelidik mengkaji tingkah laku bahan komposit diperkukuhkan dengan gentian pendek. Karya ini mengkaji kesan kedudukan gentian pendek kepada jumlah kekukuhan bahan komposit diperkukuhkan dengan nanotube karbon untuk pelbagai pecahan kelantangan. Tiga situasi yang berbeza telah dicadangkan untuk jawatan serat CNT berkenaan dengan gentian lain dalam rencam: serat sepenuhnya dipisahkan, gentian dengan pertindihan, dan serat berhubung melalui nod yang dikongsi (serat panjang). Tiga kes yang berbeza termasuk kes di mana hanya bertindih dibenarkan, kes apabila hanya serat panjang yang dibenarkan dan kes di mana kedua-dua pertindihan dan serat panjang dibenarkan telah disiasat. Ia telah menunjukkan bahawa kesan daripada kes-kes pada modulus Young rencam adalah penting dan mereka perlu dipertimbangkan untuk pemahaman yang lebih baik daripada tingkah laku komposit bertetulang. Di samping itu, ia menunjukkan bahawa kesan daripada kes yang disiasat adalah lebih luar biasa pada nombor yang lebih tinggi nilai-nilai rawak.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

LIST OF SYMBOLS

V_f	Fibers volume fraction
E	Young's modulus
D_t	Tube diameter
R_{vdw}	Closest distance between walls
E_o	Longitudinal Young's modulus
m	Matrix
f	Fiber

CHAPTER 1

INTRODUCTION

1.1 Introduction

This chapter consists of several sections which are considered as preparation to start the main research on evaluation of the influence of different arrangements of carbon nanotube fibers and volume fractions on the mechanical properties of composite materials reinforced with carbon nanotubes. The first section is the background of the study which contains definitions of some key concepts, the objective of the study and finally, the scopes of the research.

In this study, the mechanical properties of carbon nanotube reinforced composites under tensile load are going to be investigated using the finite element method provided in the commercial software MSC.Marc.

1.2 Background of the Study

1.2.1 Composites

A composite is a structural material that consists of two or more combined constituents that are combined at a macroscopic level and are not soluble in each other. One constituent is called the reinforcing phase and the one in which it is embedded is called the matrix. The reinforcing phase material may be in the form of fibers, particles, or flakes. The matrix phase materials are generally continuous. Examples of composite systems include concrete reinforced with steel and epoxy reinforced with graphite fibers, etc.[1].

1.2.2 Composites classification

Composites can be classified based on the geometry of their reinforcements and type of their matrix phase. Based on the geometry of the reinforcements, we can classify composites as particle composites, flake composites and fiber composites. On the other hand, based on the type of matrix, a composite can be a polymer, metal, ceramic or carbon composite.

1.2.3 Fiber Composite

Composites are classified by the geometry of the reinforcements (particle, flake, and fibers) or by the type of matrix (polymer, metal, ceramic, and carbon).

Fiber composites consist of matrices reinforced by short (discontinuous) or long (continuous) fibers. Fibers are generally anisotropic and examples include carbon and aramids. Examples of matrices are resins such as epoxy, metals such as aluminum, and ceramics such as calcium-alumino silicate [1].

1.2.4 Fibers classification/orientation

The reinforcement phase of a fiber composite may consist of continuous (long fibers) and aligned fibers, discontinuous (short fibers) and aligned fibers or discontinuous and randomly oriented fibers (Figure 1.1).

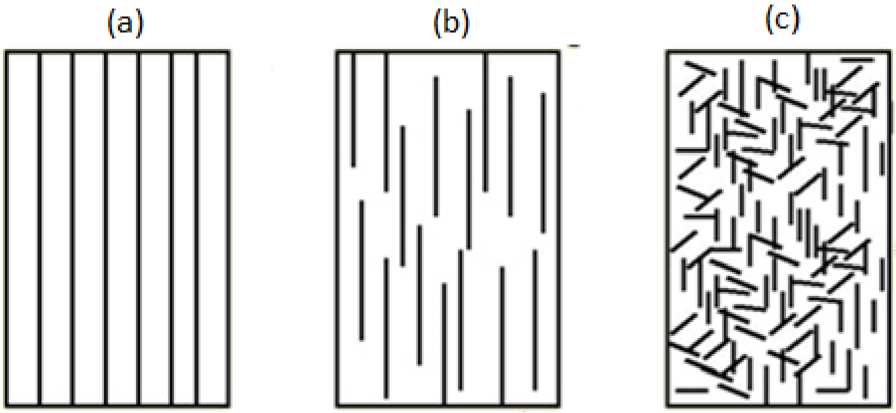

Figure 1.1 Fibers classification/orientation. (a) continuous (long fiber) and aligned fibers, (b) discontinuous (short fiber) and aligned fibers and (c) discontinuous and randomly oriented fibers.

1.2.5 Nanocomposites

Nanocomposites consist of materials that are of the scale of nanometers (10^{-9} m). Whenever at least one of the constituents of a composite is less than 100 nm, it can be classified as a nanocomposite. At this scale the properties of the materials are different from those of the bulk material. Applications of nanocomposites include packaging applications for the military in which nanocomposite films show improvement in properties such as elastic modulus and transmission rates for water vapor, heat distortion, and oxygen[1].

1.2.6 Carbon nanotubes

The modern world desires new technologies which are based on new thoughts toward science separated into several categories, for example, from medicine to aerospace. These new technologies require new tools created by novel materials; these are critical to industry because of some of their outstanding properties. Carbon nanotubes (CNTs) are a kind of these novel materials in which their applications are emerging day-to-day. CNTs are molecular-scaled cylindrical hollow structures that were first discovered by Iijima in 1991 [2]. Lightness, high toughness and strength are examples of their superior properties. These properties made them popular and they have been used as reinforcements for polymer, ceramic and metal composites.

Many researchers have been studying on finding and improving the properties of CNTs. Most of these studies predict Young’s modulus of about 1TPa and tensile strengths of up to 63 GPafor CNTs [3].

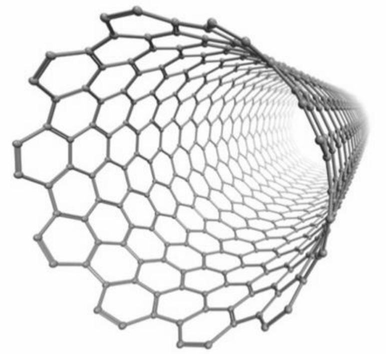

Figure 1.2 Carbon nanotube*(Artwork by futuretimeline.net)*

There are two kinds of carbon nanotubes, single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs). Single-walled carbon nanotubes can be produced by rolling a graphene sheet to a hollow cylinder or tube created from carbon atoms with only one atom in thickness [4, 5], while a multi-walled carbon nanotube is the result of combination of 2 or more (up to 50) concentric and coaxial single-walled carbon nanotubes with an inter-layer spacing of 0.34 nm[6] (Figure 1.3).

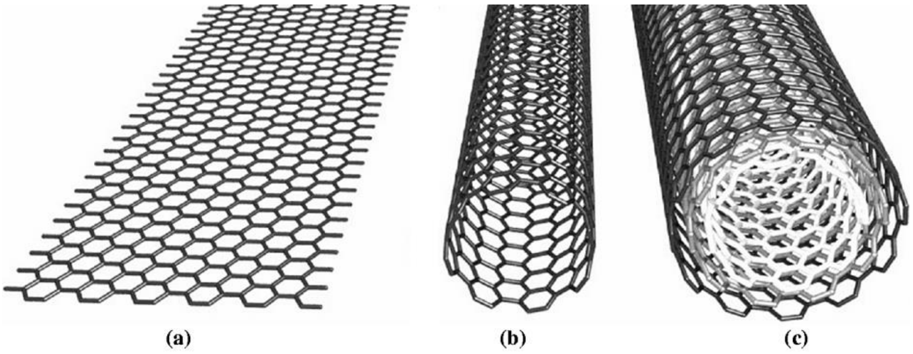

Figure 1.3 (a) Graphene sheet, (b) single-walled carbon nanotube, (c) multi-walled carbon nanotube [7].

1.2.7 Representative Volume Element

A representative volume element (RVE) is the smallest material volume element of the composite which can represent the behavior of the whole composite sufficiently accurate.

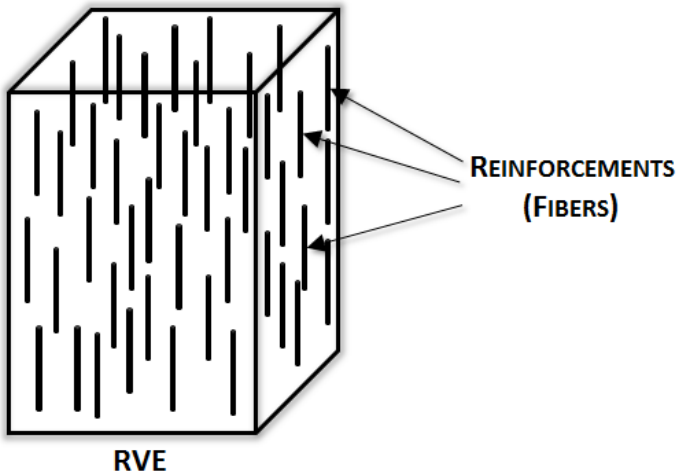

Figure 1.4 Representative Volume Element (RVE)

1.2.8 Volume Fraction

Volume fraction is the total volume of all the fibers within a composite materialdivided by the total volume of the composite. It can be shown in percentage, which means the percentage of the volume of fibers distributed in a composite over the total volume of it.

$$V_f(\%) = \frac{Volume_{Fibers}}{Volume_{Total}} \times 100 \qquad (1\text{-}1)$$

Where, V_f is the volume fraction, $Volume_{Fibers}$ is the total volume of the distributed fibers and $Volume_{Total}$ is the total composite volume (including the fibers and the matrix).

1.2.9 Position of Fibers

When distributing parallel nanotubes in a composite, there are three possibilities for positioning the nanotubes with respect to each other. They may be simply separated from each other, be connected to other nanotubes through a shared node (long fiber) or they may have certain overlaps with others (see Figure 1.5).

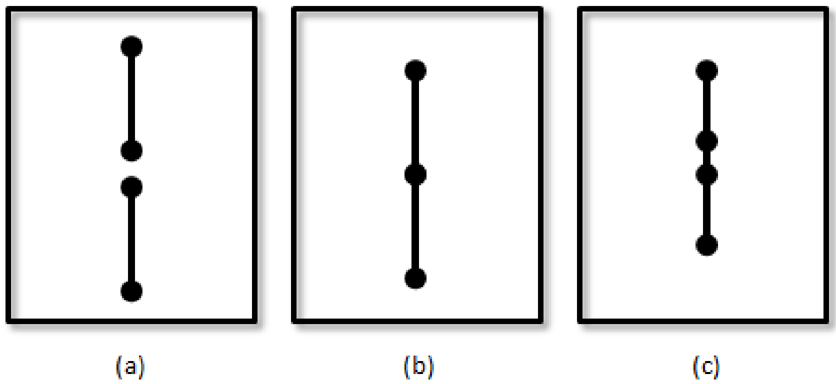

Figure 1.5(a) Completely separated fibers, (b) fibers with a shared node (connected fibers), (c) overlapping fibers.

1.2.10 Effective Area

Effective area is the cross-section area of the composite. Modeling a fiber reinforced composite in a FE software requires defining the fibers, for example, as rod (2D) elements and the matrix as 3D brick (solid) elements. Figure 1.6 shows a RVE with four fibers distributed in it. Since fibers are 2D line elements in our approach, they donot have any cross section area that can be seen, but in the pre-processing section of the FEA program,when introducing the geometry properties of these elements, the cross-section area must be defined, so although the cross-section area of these elements cannot be seen in the model, it exists and must be considered in final calculations.

Effective Area = Matrix cross-section area + Fibers cross-section area (1-2)

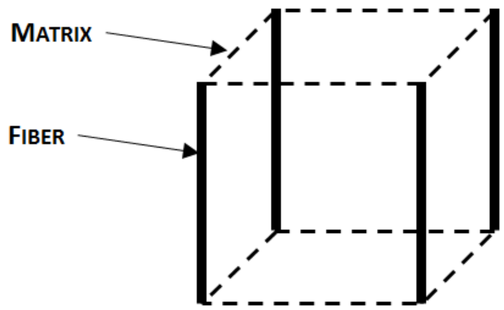

Figure 1.6 An RVE with four fibers distributed in it.

1.2.11 Finite Element Method

The finite element method (FEM) is one of the most powerful tools among the numerical approximate methods. The key idea is to use a finite number of elements in order to analyze a problem. The process consists of three main parts. Pre-processing which involves creating the model, defining the geometric and material properties, choosing the appropriate element type based on the problem and the desired results, and applying the necessary boundary conditions; the processing phase in which the system of equations is solved, and finally, the last step is called post-processing. Post-processing refers to all the tools that could be used to export the obtained results from the processing step.

There are many companies working on developing FEM software packages, among them are ANSYS (ANSYS), DassaultSystemes (Catia, Abaqus, …), MSC Software (MSC Nastran, MSC Marc, …), etc.

1.3 Statement of the Problem

Since the consideration of materials in nano scale is very difficult and time consuming, using a numerical method (finite element) is required.

The purpose of this study is to simulate the behaviour of composite materials reinforced with carbon nanotubes in order to find the mechanical properties of them, such as Young’s modulus and Poisson’s ratio. For this, MSC Marc which is a FEA software has been used.

Many researches have been done to anticipate the elastic properties of this kind of composite materials (short fiber reinforced composites). The aim of the actual research is to continue these works and to offer a more realistic modeling by considering three different cases of fiber arrangement: completely separated fibers (as in the previous work), fibers with overlap, and fibers connected through a shared node (long fibers). This consideration of different fiber positions is much closer to real distributions and allows a more accurate prediction of the macroscopic properties of the composite material.

1.4 Objective and Scopes of theStudy

1.4.1 Objective

To determine the mechanical properties of CNT reinforced composites for different randomness / arrangements of the tubes and volume fractions.

1.4.2 Scopes of the Study

- Literature Review of previous studies
- Generation of appropriate computational model

- Simulation of tensile test to predict the Young's modulus and Poisson's ratio of CNT reinforced composites
- Evaluation and Documentation

REFERENCES

1. Kaw, A.K., *Mechanics of Composite Materials, Second Edition*. 2006: Taylor & Francis.

2. Iijima, S., *Helical microtubules of graphitic carbon.* Nature, 1991. **354**(6348): p. 56-58.

3. Harris, P.J.F., *Carbon nanotube composites.* International Materials Reviews, 2004. **49**(1): p. 31-43.

4. Zhang, H.W., J.B. Wang, and X. Guo, *Predicting the elastic properties of single-walled carbon nanotubes (vol 53, pg 1929, 2005).* Journal of the Mechanics and Physics of Solids, 2005. **53**(12): p. 2794-2794.

5. Rakesh Prabu, T., *Finite Element Modeling Of Multiwalled Carbon Nanotube*, 2010, National institute of technology Rourkela.

6. Rahmandoust, M. and A. Öchsner, *Influence of Structural Imperfections and Doping on the Mechanical Properties of Single-Walled Carbon Nanotubes.* Journal of Nano Research, 2009. **6**: p. 185-196.

7. Kreupl, F., et al., *Carbon nanotubes for interconnect applications.* Ieee International Electron Devices Meeting 2004, Technical Digest, 2004: p. 683-686.

8. Fukuda, H. and K. Kawata, *On Young's modulus of short fibre composites.* Fibre Science and Technology, 1974. **7**(3): p. 207-222.

9. Tandon, G.P. and G.J. Weng, *The effect of aspect ratio of inclusions on the elastic properties of unidirectionally aligned composites.* Polymer Composites, 1984. **5**(4): p. 327-333.

10. Ferrari, M. and G.C. Johnson, *Effective elasticities of short-fiber composites with arbitrary orientation distribution.* Mechanics of Materials, 1989. **8**(1): p. 67-73.

11. Papathanasiou, T.D., M.S. Ingber, and D.C. Guell, *Stiffness enhancement in aligned, short-fibre composites: A computational and experimental investigation.* Composites Science and Technology, 1995. **54**(1): p. 1-9.

12. S. B. Sinnott, O.A.S., C. T. White and D. W. Brenner, *Mechanical properties of nanotubule fibers and composites determined from theoretical calculations and simulations.* Carbon, 1998. **36**: p. 1-9.

13. Hsueh, C.-H., *Young's modulus of unidirectional discontinuous-fibre composites.* Composites Science and Technology, 2000. **60**(14): p. 2671-2680.

14. Odegard, G.M., et al., *Constitutive modeling of nanotube-reinforced polymer composites.* Composites Science and Technology, 2003. **63**(11): p. 1671-1687.

15. Fukuda, H. and Y. Takao, *1.13 - Thermoelastic Properties of Discontinuous Fiber Composites*, in *Comprehensive Composite Materials*, K. Editors-in-Chief: Anthony and Z. Carl, Editors. 2000, Pergamon: Oxford. p. 377-401.

16. Thostenson, E.T. and T.W. Chou, *On the elastic properties of carbon nanotube-based composites: modelling and characterization.* Journal of Physics D-Applied Physics, 2003. **36**(5): p. 573-582.

17. Chen, Y.J.L.a.X.L., *Continuum Models of Carbon Nanotube-Based Composites Using the Boundary Element Method.* Electronic Journal of Boundary Elements, 2003. **1**(2): p. 316-335.

18. Liu, Y.J., N. Nishimura, and Y. Otani, *Large-scale modeling of carbon-nanotube composites by a fast multipole boundary element method.* Computational Materials Science, 2005. **34**(2): p. 173-187.

19. Eslami Afrooz, I., A. Öchsner, and M. Rahmandoust, *Effects of the carbon nanotube distribution on the macroscopic stiffness of composite materials.* Computational Materials Science, 2012. **51**(1): p. 422-429.

20. *Help, Getting started, Mathworks MATLAB R2013a.*

21. *Help. User's guide. Introduction. MSC Marc. 2012.*

22. *Help. Volume B. Element Library. MSC Marc 2012.*