

NUMERICAL INVESTIGATION OF COMPOSITE MATERIALS  
REINFORCED WITH CARBON NANOTUBES WAVINESS

MORTEZA FARSADI

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

DECEMBER 2010

Specially dedicated to my beloved mother, father, sister and brother

For all their endless moral and financial support

## ACKNOWLEDGEMENT

This thesis would not be complete without tanking everyone that helped me and supported me for the last two years. It is impossible to put into words my gratitude to all of you, so, please, excuse me if I am not able to transmit my appreciation in these few lines.

First to my supervisor, Professor Dr.-Ing. Andreas Öchsner, who has not only been the most effective anchor during my research, but also a true colleague in this endeavor, thank you for your guidance and especially for your positiveness and support when results were elusive. Thank you for believing in this project and in me, and for everything I have learnt from you. Your dedication, motivation, and insight have been fundamental in the success of this project. I wish you all the best in the future.

Second, to the people who worked with me at different points of the research, thank you for your motivation and insight: to F. Salimi, A. Sarkheyli, J. Kashani, M. Eslami, and E. Akbari. This would not have been possible without your work and dedication.

Next, I would like to thank the people who had to deal with me every day (and some nights), my lab mates: Moones Rahmandoust, Hamid Mozafari, Iman

Eslami, Meysam Hassani. Thank you all for the support and advice, the hard work and the laughs we shared.

To my friends, here, in Malaysia, and around the world, especially in Iran, thank you for your constant support at every moment. Thank you for never letting me down.

To my family, who has been behind me from the very beginning and supported me when I decided to completely change my life. Thank you for your love and support through the years and for letting me live my dream.

Last, and most importantly, I want to thank the Lord my God, who has given me both the ability and opportunity – undeserving – to live my dreams.

## ABSTRACT

Regarding thermal, mechanical and electrical properties, substantial prospective advances have been offered by Nanotube-reinforced polymers in comparison with pure polymers. This project studies the extent to which the effective stiffness of these materials can be influenced by the characteristic waviness of nanotubes embedded in polymers. In order to numerically determine how the mechanical properties of composite materials which are reinforced with carbon nanotube, are affected by nanotube waviness, a 3D element model of sinusoidal is applied. According to the obtained results, nanotube waviness causes a decrease in the effective modulus of the composite compared to the straight nanotube reinforcement. The degree to which this decrease happens depends on the ratio of the sinusoidal wavelength to the nanotube diameter. It is indicated from these results that nanotube waviness can be another mechanism which limits the modulus improvement of nanotube-reinforced polymers. Several different meshes have been applied on the model in order to predict its effect on the mechanical properties of composite. The results show that finding a proper mesh has significant role in evaluating the model.

## ABSTRAK

Mengenai sifat termal, mekanika dan elektrik, pendekatan substansial yang maju telah ditawarkan dengan polimer nanotube reinforced dengan diperbandingkan bersama polimer asli. Pengajian projek ini untuk mengkaji sejauh mana keberkesanan daripada bahan tersebut boleh dipengaruhi oleh ciri-ciri waviness nanotubes yang tertanam dalam polimers. Dalam keadah berangka untuk menentukan bagai mana sifat mekanik bahan komposit yang diperkuat dengan nanotube karbon, yang dipengaruhi oleh sifat waviness nanotube, model elemen 3D sinusoidal telah diterapkan untuk aplikasinya. Berdasarkan keputusan yang diperolehi, waviness nanotube menyebabkan penurunan modulus berkesan daripada komposit dibandingkan kepada penguatan nanotube lurus. Sejauh mana ia menurun, bergantung kepada nisbah daripada panjang gelombang sinusoidal dengan diameter nanotube. Hal ini ditunjukkan dari hasil yang waviness nanotube ini boleh menjadi mekanisme lain yang menyekat peningkatan modulus polimer nanotube reinforced. Beberapa cara mesh berbeza telah dilaksanakan pada sifat mekanik komposit. Keputusan kajian menunjukkan bahawa cara mencari mesh yang tepat merupakan peranan yang utama dalam menilai model dalam kajian ini.

**TABLE OF CONTENTS**

<b>CHAPTER</b>	<b>TITLE</b>	<b>PAGE</b>
	<b>DECLARATION</b>	ii
	<b>DEDICATION</b>	iii
	<b>ACKNOWLEDGEMENT</b>	iv
	<b>ABSTRACT</b>	vi
	<b>ABSTRAK</b>	vii
	<b>TABLE OF CONTENTS</b>	viii
	<b>LIST OF TABELS</b>	xii
	<b>LIST OF FIGURES</b>	xiii
	<b>LIST OF SYMBOLS</b>	xviii
	<b>LIST OF ABBREVIATION</b>	xx
	<b>LIST OF APPENDICES</b>	xxi
<b>1</b>	<b>INTRODUCTION</b>	1
	1.1 Background of Carbon nanotubes (CNTs)	1
	1.2 Objectives of the Project	4
	1.3 Scopes of the Project	5
	1.4 Problem Statement	5

<b>2</b>	<b>LITERATURE REVIEW</b>	<b>7</b>
2.1	Introduction	7
2.2	Structure of Carbon Nanotubes	10
2.2.1	Semiconducting and Metallic Carbon Nanotubes	13
2.3	Mechanical Properties of Carbon Nanotubes	14
2.3.1	Elastic Behavior of CNTs	15
2.4	Short Fiber	21
2.5	Curved Fiber	25
2.6	Elastic Moduli	28
2.6.1	Definition of Stress	29
2.6.2	Definition of Strain	30
2.6.3	Axial Stresses	32
2.6.4	Hooke's Law	34
<b>3</b>	<b>METHODOLOGY</b>	<b>36</b>
3.1	Introduction	36
3.2	Finite Element Methods	37
3.3	Introduction of SolidWorks Software	38
3.4	Introduction of FEMAP Software	39
3.5	Introduction of MARC Mentat Software	40
3.6	Process of Research	41
3.7	Procedure of research	42
3.7.1	Pre-Processing	42
3.7.2	Processing	45
3.7.3	Post-Processing	46
3.1	Operational Framework	47

<b>4</b>	<b>DATA and ANALYSIS</b>	<b>49</b>
4.1	Introduction	49
4.2	Definition of Model	50
4.2.1	Uniform Fiber Waviness Model	50
4.3	Finite Element Modeling	51
4.3.1	Solid Works Software	52
4.3.1.1	Straight Fiber	52
4.3.1.2	The Fiber Waviness of 0.08	54
4.3.2	Femap Software	58
4.3.2.1	The Model with 630 Nodes	58
4.3.2.2	The Model with 1287 Nodes	60
4.3.2.3	The Model with 2288 Nodes	61
4.3.3	MSC Marc Software	65
4.3.3.1	Material Properties	65
4.3.3.2	Boundary Condition	66
4.3.3.3	Link	68
4.3.3.4	Results	69
4.4	Analyzing	71
4.4.1	Young's Modulus ( $E$ )	74
4.4.1.1	Parallel ( $E_{11}$ )	75
4.4.1.2	Perpendicular ( $E_{22}$ )	77
4.4.2	Poisson's Ratio ( $\nu$ )	78
4.4.2.1	Parallel	82
4.4.2.2	Perpendicular	84
4.5	Validation	85
4.5.1	Finite Element Analysis	86

<b>5</b>	<b>RESULTS and DISCUSSION</b>	<b>91</b>
	5.1 Introduction	91
	5.2 Results and Discussion	93
	5.2.1 Waviness Ratio ( $w = a/L$ )	93
	5.2.1.1 Young's Modulus ( $E$ )	93
	5.2.1.2 Poisson's Ratio ( $\nu$ )	95
	5.2.2 Number of Nodes	99
	5.2.3 Volume Fraction ( $V_f$ )	102
	5.2.3.1 Young's Modulus ( $E$ )	103
	5.2.3.2 Poisson's Ratio ( $\nu$ )	106
<b>6</b>	<b>Conclusion and Recommendation</b>	<b>109</b>
	6.1 Introduction	109
	6.2 Conclusion	110
	6.3 Future Work	110
	<b>REFERENCE</b>	<b>112</b>
	<b>APPENDIX</b>	<b>119</b>

## LIST OF TABLES

TABLE NO.	TITLE	PAGE
1.1	Comparison of mechanical properties of same popular composites and metals.	3
2.1	Types of nanotubes based on chiral indices.	11
2.2	Commonly referenced mechanical properties of CNTs ( $\varnothing_{int}$ and $\varnothing_{ext}$ correspond to inner and outer diameter respectively).	19
2.3	Comparison of mechanical properties of CNTs, Carbon, and Kevlar fibers and high-tensile steel. The values for the CNT were taken for a SWCNT of diameter 10 nm, using the entire area enclosed by the tube to normalize stiffness/strength.	20
2.4	Experimental stress-strain data for a variety of glass/epoxy systems.	22
4.1	Fiber and matrix of model separately.	56
4.2	Assembly of model.	57
4.3	The other models which are used in the project.	63
4.4	The model with 2288 nodes in 4 different volume fractions.	64

**LIST OF FIGURES**

<b>FIGURE NO.</b>	<b>TITLE</b>	<b>PAGE</b>
1.1	Specific strength and stiffness of some popular composites and metals.	4
2.1	Roll-up vectors defining the structure of Carbon nanotubes. (a) Graphene lattice and (b) Carbon nanotube.	11
2.2	Zig-zag, chiral and armchair nanotubes and their corresponding caps.	12
2.3	Conductivity roadmap for SWCNTs indicating the conductivity of the nanotube produced with a chiral vector of given $(n,m)$ integers.	14
2.4	Images of nanotube-reinforced polymers (a) TEM image of MWNTs (1wt.%) in polystyrene. (b) SEM image of MWNTs (50 wt. %) in poly (vinyl alcohol).	15
2.5	Specific strength vs. specific modulus for the most common materials compared to CNTs. Chart modified from Ashby's plots.	21
2.6	Schematic of laminate analogy for predicting mechanical properties of 2-dimensional short fiber composite.	24

2.7	Effects of fiber aspect ratio, fiber volume fraction, and fiber-to-matrix stiffness ratio on the longitudinal stiffness of unidirection-ally oriented, short glass fiber/epoxy composites.	25
2.8	Definitions of tensile stress $\sigma$ .	29
2.9	Definitions of tensile strain.	31
2.10	A plate loaded in tensile.	34
3.1	(a) carbon nanotube, (b) equivalent continuum model, (c) effective fibre, and (d) 3D element fibre.	41
3.2	Schematics of models to evaluate effective mechanical properties of Nanotube composite: (a) nanocomposite; (b) coordinate systems.	43
3.3	Operational framework.	48
4.1	Representative volume element (RVE) and coordinates for a unidirectional composite with graded waviness.	51
4.2	Fundamental model of composite reinforced with carbon nanotube: (a) Fiber; (b) matrix; (c) assembly model.	53
4.3	Fundamental model of composite reinforced with carbon nanotube: (a) Fiber; (b) matrix; (c) assembly model.	54
4.4	Model with straight fiber: (a) meshed fiber; (b) meshed matrix.	59
4.5	Model with 0.08 waviness ratio of fiber: (a) meshed fiber; (b) meshed matrix.	59
4.6	Model with straight fiber: (a) meshed fiber; (b) meshed matrix.	60
4.7	Model with 0.08 waviness ratio of fiber: (a) meshed fiber; (b) meshed matrix.	61
4.8	Model with straight fiber: (a) meshed fiber; (b) meshed matrix.	62

4.9	Model with 0.08 waviness ratio of fiber: (a) meshed fiber; (b) meshed matrix.	62
4.10	Materials of the model mentioned above.	66
4.11	Boundary condition of the model where the parallel force is exerted to the fiber.	67
4.12	Boundary condition of the model where force is exerted perpendicular to the fiber.	67
4.13	(a) A model linked parallel to the fiber (b) A model linked perpendicular to the fiber.	69
4.14	Model resizing under parallel force.	70
4.15	Model resizing under the perpendicular force.	70
4.16	Dimension of the selected model.	72
4.17	The force in the fiber direction (a) full view of the selected model (b) $x$ - $y$ plane (c) $x$ - $z$ plane (d) $y$ - $z$ plane.	79
4.18	The force in perpendicular direction to the fiber (a) full view of the selected model (b) $x$ - $y$ plane (c) $x$ - $z$ plane (d) $y$ - $z$ plane.	80
4.19	Schematic of the finite element cell model of an embedded wavy nanotube. For the particular model shown $w = a/L = 0.01$ and $(L/d) = 100$ .	86
5.1	Illustrative example of evaluating nanotube waviness.	92
5.2	Young's modulus ( $E$ ) as a function of nanotube waviness ratio ( $w = a/L$ ) for different meshes where the displacement is applied in the longitudinal direction (for a volume fraction $V_f = 0.014$ ).	94
5.3	Young's Modulus ( $E$ ) as a function of nanotube waviness ratio ( $w = a/L$ ) for different meshes where the displacement is applied in the transverse direction (for a volume fraction $V_f = 0.014$ ).	95
5.4	Poisson's ratio $\nu_{yx}$ as a function of waviness parameter $w = a/L$ for three cases of meshing where the displacement is applied in the longitudinal direction (for volume fraction $V_f = 0.014$ ).	96

5.5	Poisson's ratio $\nu_{yz}$ as a function of waviness parameter $w = a/L$ for three cases of meshing where the displacement is applied in the longitudinal direction (for volume fraction $V_f = 0.014$ ).	97
5.6	Poisson's ratio $\nu_{yx}$ as a function of waviness parameter $w = a/L$ for three cases of meshing when the displacement is applied in the transverse direction (for volume fraction $V_f = 0.014$ ).	98
5.7	Poisson's ratio $\nu_{yz}$ as a function of waviness parameter $w = a/L$ for three cases of meshing where the displacement is applied in the transverse direction (for volume fraction $V_f = 0.014$ ).	99
5.8	Effect of meshing on the Young's modulus ( $E$ ) values calculated by FEM simulation for different nanotubes waviness ratios ( $w = a/L$ ) where the displacement is applied in the longitudinal direction (for volume fraction $V_f = 0.014$ ).	101
5.9	Effect of meshing on the Young's modulus ( $E$ ) values calculated by FEM simulation for different nanotubes waviness ratios ( $w = a/L$ ) where the displacement is applied in the transverse direction (for volume fraction $V_f = 0.014$ ).	102
5.10	Young's modulus ( $E$ ) as a function of nanotube waviness ratio ( $w = a/L$ ) for different volume fractions ( $V_f$ ) where the displacement is applied in the longitudinal direction (With 2288 Nodes).	103
5.11	Young's modulus ( $E$ ) as a function of nanotube waviness ratio ( $w = a/L$ ) for different volume fraction ( $V_f$ ) where the displacement is applied in the longitudinal direction (With 2288 Nodes).	105

- 5.12 Poisson's ratio  $\nu_{yx}$  as function of volume fraction ( $V_f$ ) 106  
for different nanotube waviness ratios ( $w = a/L$ )  
where the displacement applied in the longitudinal  
direction (With 2288 Nodes).
- 5.13 Poisson's ratio  $\nu_{yz}$  as function of volume fraction ( $V_f$ ) 107  
for different nanotube waviness ratios ( $w = a/L$ )  
where the displacement is applied in the longitudinal  
direction (With 2288 Nodes).

## LIST OF SYMBOLS

SYMBOL	DISCRIPTION
$^{\circ}\text{C}$	Degree celcius
$C_h$	Chiral vector
$\theta$	Chiral angle
$a_1, a_2$	Vectors of the hexagonal graphite lattice
$R_{NT}$	Radius of any nanotube
$E$	Young's modulus
$\sigma_f$	Fracture stress
$\sigma_y$	Yield stress
$E^b$	Bending elastic modulus of a CNT
$E^a$	Axial elastic modulus of a CNT
$E^w$	Wall elastic modulus of a CNT
$\varnothing_{int}$	Diameter of the inner wall of a MWCNT
$\varnothing_{ext}$	Diameter of the outer wall of a MWCNT
$F$	Force
$\sigma$	Tensile stress
$\sigma_{nom}$	Nominal stress
$A$	Cross section
$\Delta L$	Displacement
$L$	Initial length
$\nu$	Poisson's ratio

$\varepsilon_t$	Tensile strain
$\varepsilon_l$	Lateral Strain
$d$	Diameter on nanotube (NT)
$L$	Wavelength of the NT waviness
$a$	Amplitude of the NT waviness
$w$	Fiber waviness ratio
$V_f$	Volume fraction of fiber
$V_m$	Volume fraction of matrix
$E_m$	Young's modulus of matrix
$E_{CNT}$	Young's modulus of fiber (CNT)
$\nu_m$	Poisson's ratio of matrix
$\nu_{CNT}$	Poisson's ratio of fiber (CNT)
$A_{CNT}$	Sectional area of the fiber (CNT)
$A_{matrix}$	Area of matrix
$A_{composite}$	Area of composite
$\Sigma F$	Sum of reaction forces
$E_{11}$	Longitudinal Young's modulus
$E_{22}$	Transverse Young's modulus
$\nu_{yx}$	Poisson's ratio in y-x plane
$\nu_{yz}$	Poisson's ratio in y-z plane
$\varepsilon_x$	Strain in x direction
$\varepsilon_y$	Strain in y direction
$\varepsilon_z$	Strain in z direction
$\Delta L_x$	Displacement of x direction
$\Delta L_y$	Displacement of y direction
$\Delta L_z$	Displacement of z direction
$E_{cell}^{FEA}$	Effective modulus of the cell
$E_{ERM}$	Effective reinforcing modulus
$E_{ratio}$	Ratio of CNT modulus and matrix modulus
$\eta$	Percentage of error

## LIST OF ABBREVIATIONS

CNT	Carbon Nanotube
ESD	Dissipation of electrostatic charge
SWCNT	Single Wall Carbon Nanotube
MWCNT	Multi Wall Carbon Nanotube
AFM	Atomic Force Microscopy
TEM	Transmission Electronic microscopy
FE	Finite Element
FEM	Finite Element Method
NT	Nanotube
FEA	Finite Element Analysis
RVE	Representative Volume Element

**LIST OF APPENDICES**

<b>APPENDIX</b>	<b>TITLE</b>	<b>PAGE</b>
1	Project Schedule in Pre-Project	119
2	Project Schedule in Final Project	120

## **CHAPTER 1**

### **INTRODUCTION**

#### **1.1 Introduction**

When a material is composed of one or more discontinuous phases incorporated in a continuous phase, it is termed a composite. The reinforced or reinforcing material (fiber) is usually termed the discontinuous phase and in comparison with the continuous phase, which is named the matrix, it is typically the harder and stronger phase. The mechanical properties of a composite have a strong dependency on the distribution of the reinforcing material, their properties and interactions with the matrix [1].

The fibers have been used as stiffening and strengthening agents since *800 BC* by ancient Egyptians who blended straw and clay to make reinforced bricks. This is one of the first documented examples in which a one dimensional, high-aspect-ratio filler was applied to produce a composite which has higher stiffness and strength compared to the matrix material. In Mongolia natives made their bows out of animal tendons, wood and silk about *1300 AD*, that is another instance of early fiber reinforced composites [2]. These and many others naturally occurring fibers for example sisal, hemp, kenaf, flax, jute and coconut were broadly employed for centuries, to create composites with improved mechanical properties. A number of natural fibers are still being in application in which recyclability of the part is vital.

Significant research has focused on Carbon nanotubes (CNTs) as fiber since their discovery by Iijima in 1991 [3]. Carbon nanotubes have exceptional mechanical properties in addition to the exceptional electronic and thermal properties related with them [4]: experimental and theoretical results which show strengths 10 to 100 times greater than the strongest steel at a fraction of the weight and an elastic modulus larger than 1 TPa, in comparison with 0.2 TPa for steel and 0.07 TPa for aluminum [5]. Because of significant mechanical properties of Carbon nanotubes, most investigators have focused on applying them as reinforcement for different materials. Reinforcement of various matrices by the use of Carbon nanotubes has become a main research interest worldwide. Due to the size of the nanotubes, the challenges related with large filler particles (especially stress concentrations) are substantially reduced. Furthermore, no other filler shows such a high strength and stiffness integrated with a low density. Lately, analytical models and extensive work on reinforcement of polymer, ceramic, and metal matrices has been developed.

Moreover, Carbon nanotubes have also been observed as reinforcement for traditional composite materials. The special mechanical properties of composite

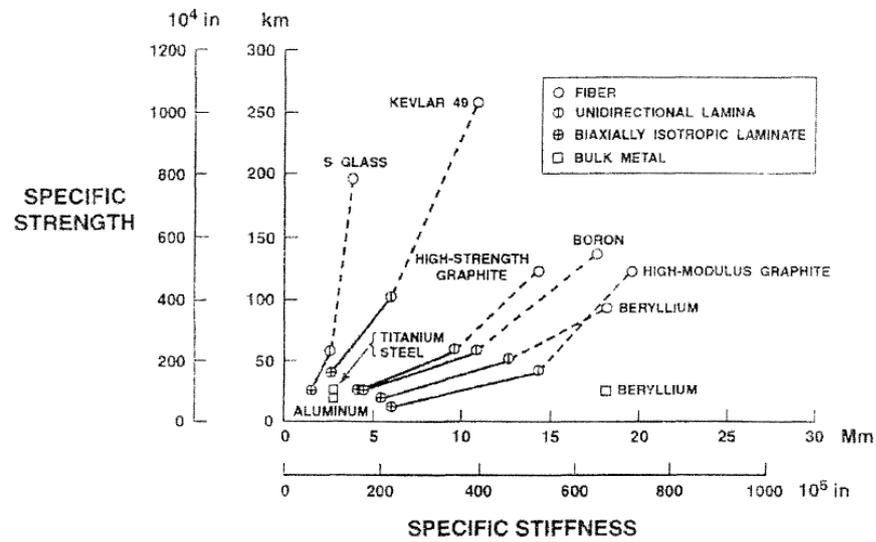
materials have allowed them to increase their presence in the aeronautical industry in the last 20 years.

Similar to the mechanical properties of the best metal alloys, composite materials have mechanical properties, but with about a third of the weight. Multilayered composite materials are efficiently used in structural parts traditionally reserved for metal alloys since they have special in-plane mechanical properties. Nevertheless, the relatively poor mechanical properties of the matrix and the fiber/matrix interfacial bond limit their use, in especially demanding applications. Table 1.1 and Figure 1.1 in which modern popular composites are compared with some typical metals in terms of their mechanical properties and density show that the interest in composites proved to be well-founded.

**Table 1.1** Comparison of mechanical properties of some popular composites and metals [6].

Material	Density (Mg/m <sup>3</sup> )	Tensile strength (GPa)	Tensile modulus (GPa)	Specific	
				Strength	Stiffness
<b>Composites<sup>d</sup></b>					
E glass	2.1	1.1	45	0.5	20
Aramid	1.4	1.4	75	1.0	90
Type I carbon	1.5	1.1	220	0.7	130
Type II carbon	2.0	1.5	140	1.0	90
<b>Metals</b>					
Steel	7.8	1.3	200	0.2	26
Aluminium	2.8	0.3	73	0.1	26
Titanium	4.0	0.4	100	0.1	25

<sup>d</sup>Sixty percent fibre volume fraction unidirectional reinforcement.



**Figure 1.1** Specific strength and stiffness of some popular composites and metals [7].

## 1.2 Objectives of the Project

The objectives of this study can be summarized as follows:

- 1) Modeling and simulation of composite material reinforced with curved fibers (Carbon nanotubes).
- 2) To determine the macroscopic mechanical properties of Carbon nanotubes reinforced composite.

### 1.3 Scopes of the Project

- 1) Generation of finite element models.
- 2) Meshing the geometry of finite elements.
- 3) Simulation of finite elements models.
- 4) To investigate the behavior for different radii of curved fibers.

### 1.4 Problem Statement

Examining the effects of misalignment or waviness got started by theoreticians about 30 years ago, despite the fact that our models of fiber composites usually have straight fibers. Therefore, expressions for the modulus of composites including random initial alignment irregularities were developed by Bolotin in 1966 [8]. He decreased these to sine waves, as later did Swift [9], who also calculated the resulting transverse forces. In addition, in discussing compressive failure of aligned fiber composites, by using a metallurgical analogy, Argon [10] showed that misalignments of fibers could initiate kinking failure in composites. Simultaneously Suarez *et al.* [11] separately came to the same conclusion in working with composite.

Davis tracked individual fibers by sequential polishing of boron/epoxy in 1974; it was the first time that actual measurements of fiber waviness were done [12]. Lately a pretty simple way to measure misalignments in unidirectional

composites was developed by Yurgarti [13], and Mrse and Piggott used this to set up a direct link between compressive strength and misalignment [14].

In this project, the Carbon nanotube (CNT) is modeled as a sinusoidal fiber which is obtained directly from a finite element approach. This approximates the NT and the surrounding matrix as a continuum; in the paper whose results have been used in this work the nature of this assumption and its limitations and justification are discussed [15].

The main purpose of this work is to develop a macromechanics-based model that can be used to assess the effect of nanotube waviness on the mechanical properties of composite materials reinforced with carbon nanotube.