NUMERICAL INVESTIGATION OF COMPOSITE MATERIALS REINFORCED WITH CARBON NANOTUBES WAVINESS

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

For all their endless moral and financial support

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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 terma, 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 cirri-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.

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LIST OF SYMBOLS

SYMBOL	DISCRIPTION
°C	Degree celcius
C_h	Chiral vector
θ	Chiral angle
a_1 , a_2	Vectors of the hexagonal graphite lattice
R_{NT}	Radius of any nanotube
E	Young's modulus
σ_f	Fracture stress
σ_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
$Ø_{int}$	Diameter of the inner wall of a MWCNT
$Ø_{ext}$	Diameter of the outer wall of a MWCNT
F	Force
σ	Tensile stress
σ_{nom}	Nominal stress
A	Cross section
ΔL	Displacement
L	Initial length
ν	Poisson's ratio

ε_t	Tensile strain
ε_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)
ν_m	Poisson's ratio of matrix
ν_{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
ΣF	Sum of reaction forces
E_{11}	Longitudinal Young's modulus
E_{22}	Transverse Young's modulus
ν_{yx}	Poisson's ratio in y-x plane
ν_{yz}	Poisson's ratio in y-z plane
ε_x	Strain in x direction
ε_y	Strain in y direction
ε_z	Strain in z direction
ΔL_x	Displacement of x direction
ΔL_y	Displacement of y direction
ΔL_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
η	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

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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 same popular composites and metals [6].

Material	Density (Mg/m^3)	Tensile strength (GPa)	Tensile modulus (GPa)	Specific	
				Strength	Stiffness
Composites[a]					
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
Metals					
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

[a] Sixty percent fibre volume fraction unidirectional reinforcement.

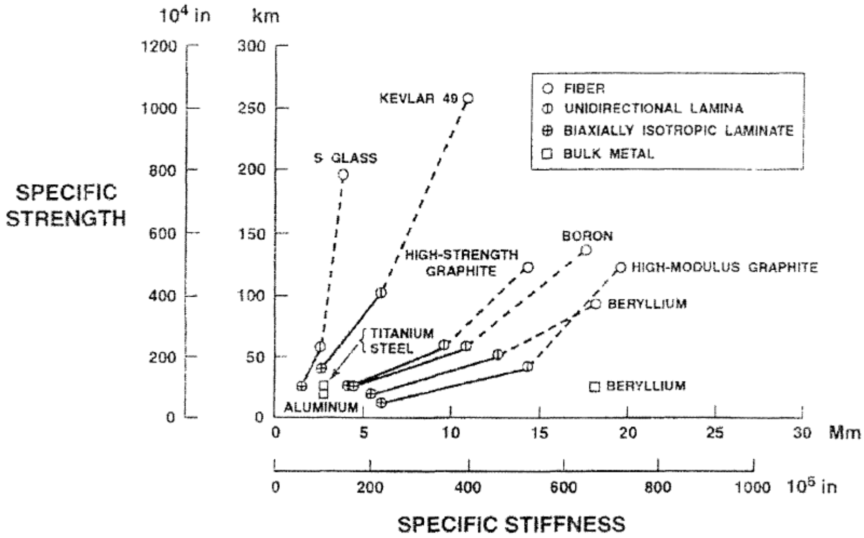

Figure 1.1 Specific strength and stiffness of some popular composites and metals [7].

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.