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Elastic response of a carbon nanotube fiber reinforced polymeric composite: A numerical and experimental study

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ABSTRACT

Premature failure due to low mechanical properties in the transverse direction to the fiber constitutes a fundamental weakness of fiber reinforced polymeric composites. A solution to this problem is being addressed through the creation of nanoreinforced laminated composites where carbon nanotubes are grown on the surface of fiber filaments to improve the matrix-dominated composite properties. The carbon nanotubes increase the effective diameter of the fiber and provide a larger interface area for the polymeric matrix to wet the fiber. A study was conducted to numerically predict the elastic properties of the nanoreinforced composites. A multiscale modeling approach and the Finite Element Method were used to evaluate the effective mechanical properties of the nanoreinforced laminated composite. The cohesive zone approach was used to model the interface between the nanotubes and the polymer matrix. The elastic properties of the nanoreinforced laminated composites including the elastic moduli, the shear modulus, and the Poisson's ratios were predicted and correlated with iso-strain and iso-stress models. An experimental program was also conducted to determine the elastic moduli of the nanoreinforced laminated composite and correlate them with the numerical values.

1. Introduction

Laminated composite materials consist of a stiff and strong micron-size phase called reinforcement, which is usually a fibrous material like a textile fabric, and another phase called matrix, which is either a polymer, a ceramic, a metal, or a carbon material. A traditional way to improve the properties of polymers and specifically increase their thermal stability and stiffness is to add micron-size fillers. However, a reduction is observed in their ductility, fracture toughness and sometimes strength. In order to avoid those property reductions, nanocomposites can be formed by dispersing nanoparticles in the polymeric matrix: platelets like clay, fibers like carbon nanotube and carbon nanofiber, or particulates like silica or expanded graphite. A considerable improvement in the mechanical properties of the polymer matrix can be achieved with small concentrations of the particles, usually less than 5% by volume. The use of these nanoparticles could however be limited by dispersion problems and viscosity build-up related to strong inter-particle interactions. The particle volume content plays a very important role but the interphase between the matrix and the particles plays an even major role. Among the nanoparticles, the best choice to improve the mechanical properties of the composites is to use carbon nanotubes due to their excellent mechanical, electrical, and thermal properties.

The discovery of fullerenes in the mid 1980s was of great importance in the development of carbon nanotubes [1,2]. Fullerenes are closed cage-like structures of carbon atoms with pentagonal and hexagonal carbon atom rings. The first fullerene was a C_{60} molecule having pentagonal carbon atom rings sharing their sides with adjacent hexagonal carbon atom rings. A few years later, a long fullerene called carbon nanotube (CNT) was first observed by Iijima [3]. Experimental studies reported an average elastic modulus of approximately 1 TPa and an average breaking strength of 30 GPa with an ultimate strain of 5.3% [4]. Other experiments also provided evidence of their high elastic modulus: approximately 1.25 TPa [5], and numerical simulations predicted similar values [6]. It is widely accepted now that CNTs possess exceptionally high mechanical, thermal and electrical properties. CNT-based composites, i.e. CNT nanocomposites, can be fabricated with a wide variety of matrix materials such as polymers, metals and ceramics. In this study, we propose to investigate a CNT nanocomposite as the matrix material of a carbon fiber reinforced polymeric composite to improve its matrix-dominated properties. The resulting nanoreinforced laminated composite is abbreviated as NRLC.

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A brief background about CNT nanocomposites, the specific objectives for the study and the multiscale modeling approach to predict the mechanical properties of the NRLC are all presented in the introduction of Section 2. The role of the interfaces in composite materials, the cohesive zone model as a tool to characterize the interface and its formulation are briefly discussed in Section 2.1. Implementation of the cohesive zone model in the Finite Element Method (FEM) and the elasticity-based solution method to evaluate the effective elastic properties of the NRLC are presented in Sections 2.2 and 2.3, respectively. The numerical results are presented in Section 3, and details of the experimental program to mechanically characterize the NRLC and its results are presented in Section 3.5, respectively. Section 4 presents the correlation between the numerical and experimental results. Finally, Section 5 provides a summary and the conclusions of this study.

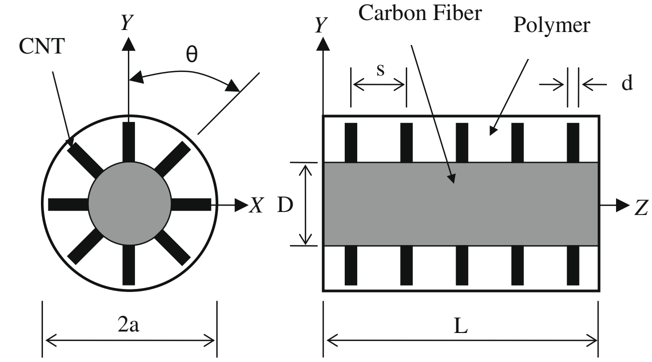

Fig. 2. Schematic illustration of an RVE of NRLC.

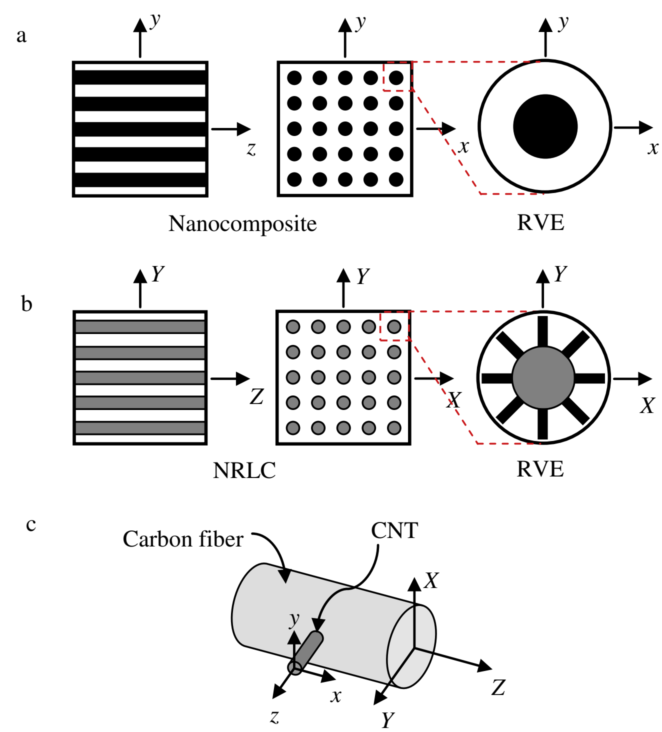

Fig. 3. Schematic illustrations of models to evaluate effective mechanical properties of NRLC: (a) nanocomposite; (b) NRLC; (c) coordinate systems.

2. Materials and numerical formulation

Chemical vapor deposition (CVD) and Nickel catalyst particles are used to grow the carbon nanotubes on the surfaces of carbon fibers [7]. Fig. 1 shows Scanning Electron Microscope (SEM) images of carbon fibers with CNTs grown on their surfaces. These fibers are then impregnated with a polymeric matrix material such as epoxy to fabricate the NRLC samples. Fig. 2 shows a schematic illustration of a representative volume element (RVE) of the NRLC. The carbon nanotubes increase the effective diameter of the fiber and provide a much larger interface area that may improve the fiber/matrix interfacial load transfer characteristics, which in turn should result in higher stiffness and strength of the nanoreinforced polymer matrix surrounding the carbon fiber. Fig. 2 shows also various geometrical parameters that can be chosen during the fabrication process.

The mechanical response of materials is governed by phenomena occurring at different scales of length and time. In nanocomposites, the interactions between the CNTs and the matrix take place at the nanoscale level but they affect the mechanical response of composites at the macroscopic level. Nanoscale phenomena are often studied by molecular dynamics (MD) simulations while behavior at the macroscopic level is conveniently studied with continuum mechanics. MD simulations are limited only to small volumes because of the intensive computational requirements. Therefore, there is a need for multiscale modeling methodologies that relate the molecular and continuum approaches.

In this study, the equivalent macroscopic or continuum-level elastic properties of the NRLC are modeled in two steps. The first step involves modeling the unidirectional nanocomposite consisting of a single CNT surrounded by the polymer matrix and predicting its overall mechanical properties (Fig. 3a). The second step requires modeling the carbon fiber nanoreinforced laminated composite (NRLC) where the matrix is the nanocomposite evaluated in the first step (Fig. 3b). It should be noted that the {*xyz*} coordinate system is used for the nanocomposite description and the {*XYZ*} coordinate system is used for the NRLC description (Fig. 3c).

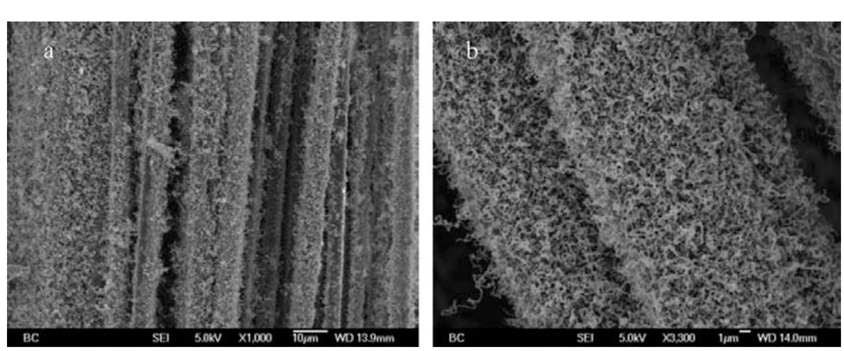

Fig. 1. SEM images of carbon fibers with CNTs grown on their surfaces: (a) fiber bundle; (b) two fibers.