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A refined analysis of the influence of the carbon nanotube distribution on the macroscopic stiffness of composites

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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.

1. Introduction

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 Ijima in 1991 [1]. 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 1 TPa and tensile strengths of up to 63 GPa for CNTs [2].

The studies on composite materials reinforced with short fibers started long time ago before discovering CNTs. These studies were done in two distinct aspects, mathematical modeling and simulating the behavior of the composites. In 1974, Fukuda and Kawata [3] proposed a mechanism for interaction between matrix and fiber under the applied load, and based on that predicted Young's modulus of short fiber reinforced materials. They assumed that the fibers have been oriented following a certain rule. They also did not consider the interaction between fibers. Based on their findings, Young's modulus of composite materials reinforced with unidirectional continuous fibers is greater than that with short fibers. Then in 1984, Tandon and Weng [4] investigated the influence of changing the aspect ratio on the effective Young's modulus of a transversely isotropic composite. They found out that the longitudinal Young's modulus increases with increasing the aspect ratio. After that, Ferrari and his colleague Johnson [5] tried to derive the effective elastic properties of composites reinforced with arbitrary oriented short-fibers using the Mori–Tanaka assumption which considers the effect of interaction between fibers and can be used for various volume fractions. In 1995, Papathanasiou et al. [6] combined computational and experimental studies to find out how the alignment of fibers can improve the effective Young's modulus. They used the boundary element method (BEM) for their computational study and a hydrodynamic method for the experimental part. They came up with the fact that aligned fibers are more effective in stiffening the composite. Sinnot et al. [7] estimated the Young's modulus for aligned single-walled carbon fibers in 1998. They used one of the properties of nanotubule fibers, that is in the limit of infinitely long tubules the fibers can have a Young's modulus near to diamond, to investigate a new carbon based composite reinforced with layered nanotubule fibers and diamond. They found out that these kinds of composites have a

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high Young's modulus, low density and can handle shear and other distortions. Then in 2000, Hsueh [8] used a modified shear-lag model to derive the Young's modulus of a unidirectional discontinuous fiber composite. The predicted Young's modulus was in good agreement with those from the Halpin–Tsai semi-empirical equation, the Eshelby model and the experimental results. In 2003, Odegard et al. [9] proposed a technique to develop constitutive models for polymer based composites reinforced with single-walled nanotubes (SWNTs). They modeled the nanotube and the nanotube/polymer interface as an effective continuum fiber by implementing an equivalent-continuum modeling method. Verified the model, they concluded that it can be applied to a range of related problems that need more accuracy of atomistic-level descriptions. Thostenson and Chon [10] continued the study on composites reinforced with carbon nanotubes by investigating existing challenges in using the carbon nanotubes properties in a macroscopic composite. They concluded that the reinforced composite elastic properties are very reliant on the nanotube diameter. Liu and Chen [11] used the BEM for their study. They focused on existing challenges in modeling the CNT-based composites including choosing the model, representative volume elements (RVEs), interface conditions, etc. They validated their results with the finite element method (FEM) and found the BEM to be a reliable tool for the analysis of composites reinforced with CNTs. Recently in 2012, Eslami and Öchsner [12] reported their study on investigating the effects of the distribution of carbon nanotubes on the stiffness of the composite using FEM. They found randomness to be one of the vital factors that must be considered in characterization of these composites. Their findings show that by increasing the randomness in distribution of fibers, the Young's modulus decreases.

However, the research by Eslami and Öchsner was limited to the simplification that the single CNTs are not in contact, i.e., completely separated fibers. The aim of the actual research is to continue this recent work 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. Other simplifications of the previous work, i.e., consideration of only parallel fibers and perfect bonding between fibers and matrix remain unchanged.

2. Modeling and simulation

The finite element method (FEM) is one of the most powerful tools among the numerical approximate methods and has been applied within this study to predict the elastic properties. Previous studies showed that nanotubes can be efficiently modeled as truss members [13] (see Fig. 1); based on this, Element 9 in the commercial code MSC.Marc, which is a line element (1D) with two nodes, has been selected to model CNTs. Also, element 7, a hexagonal solid element (3D), has been chosen to fill the composite as its matrix phase.

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 Fig. 2). Based on these arrangements, the reinforced composite Young's modulus and Poisson's ratio may change. In order to study the effect of positioning the CNTs on the elastic properties of the composite materials, several numerical tests were done, including the cases that (1) there are no overlapped or connected fibers, (2) just overlaps are allowed, (3) just long fibers are allowed and (4) both overlapped and long fibers are allowed. The obtained results are anticipated to be closer to the real world results since it is a completely random distribution of the unidirectional CNTs in a composite.

Choosing appropriate boundary conditions is one of the challenging steps in the FEM. The tensile test will be simulated in this paper. It is one of the most common methods to measure the Young's modulus of various materials. To simulate the test, the bottom surface of the RVE must be fixed in z direction and the top surface will be subjected to a uniform displacement. In order to expand the results to a bigger model, the lateral surfaces (zx and zy) of the RVE will also be fixed in y and x direction (symmetry condition), respectively (see Fig. 3).

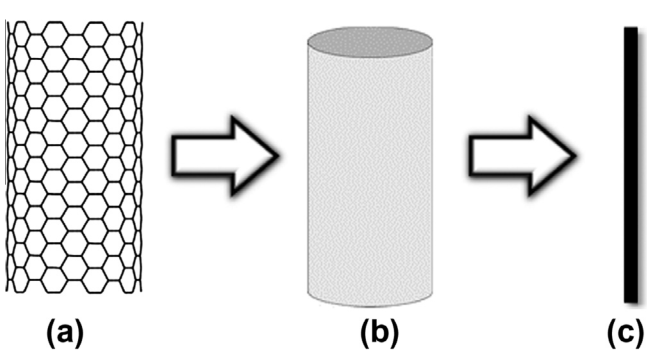

Fig. 1. (a) Carbon nanotube, (b) effective fiber and (c) truss element. Adapted from [12].

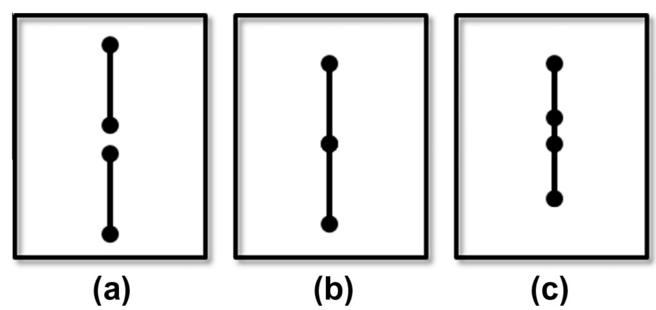

Fig. 2. (a) Completely separated fibers, (b) fibers with a shared node (connected fibers) and (c) overlapping fibers.

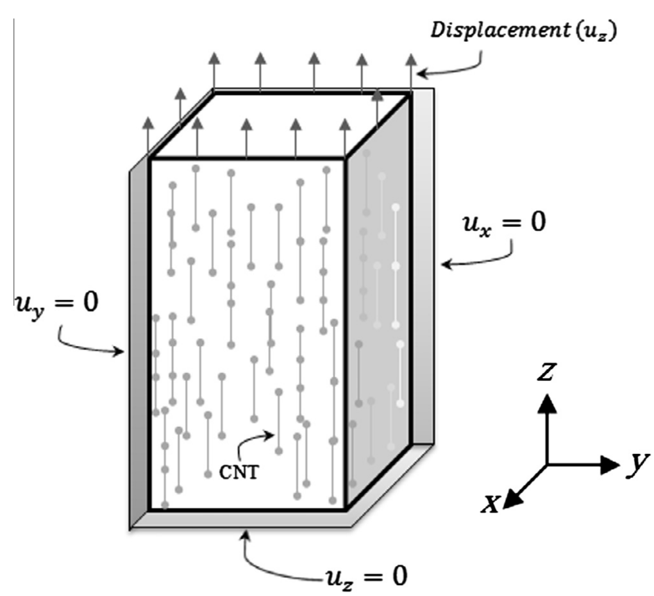

Fig. 3. Representative volume element (RVE) and the boundary conditions.