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Elastic Behavior of Carbon Nanotubes Reinforced Composites: Micromechanical Modeling

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ABSTRACT

A micromechanical model is applied to examine the tensile properties of composite materials filled with multi-wall CNT oriented in in-plane and out-of-plane direction and a quantitative micromechanical model for the mechanical behavior of CNT-composites has been developed. Digimat-MF is used to generate a realistic three-dimensional microstructure for the current carbon nanotube/ epoxy composite. The Digimat model simulates a system of aligned carbon nanotubes arranged in-plane and another one having out of plane arrangement of reinforcements. A second model shows a representative volume element for the current nano-composite, in which the carbon nanotubes were simulated as a randomly (fully) dispersed, where all particles have been separated from each other. The predicted mechanical properties are compared with experimental tensile properties of composite materials reinforced with multi-wall CNTs arranged in in-plane and out-of-plane direction. A good agreement between the micromechanical modeling and the experimental part is observed. Results show that the elastic energy stored in -the-through thickness direction reinforced composites is about two times higher than that in the pure polymer.

1. Introduction

Dramatic improvements in mechanical properties can be achieved by incorporation of a few weight percentages of layered particles in polymer matrices [1]. Layered silicates have a thickness of 1nm and lateral dimensions of 30nm to several microns are commonly used as reinforcement in polymeric based composites. The large aspect ratios of CNT are thought to be mainly responsible for the enhanced mechanical properties of particulate–polymeric based nanocomposites. On the contrary, the amazing large specific surface area of carbon nanotubes produces very large attractive forces (Vander Waals forces) between the molecules, and a tendency to agglomerate. Their tangled yarn-like structure is a further barrier to obtain specific orientation [2]. In order to transfer the superior properties of CNT into the composites and reach excellent characteristics, filler orientation need to be controlled and arranged well in the matrix, which is one of the major preconditions for the utilization of reinforcements. Epoxy

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resins on the other hand, are normally used in the formation of carbon nanotubes/ polymeric based-composites that can work as multifunctional materials with high stiffness, light weight and high electrical conductivity as well as other desired economic properties for many industrial applications [3, 4]. Epoxy resins start in a molten form to assist dispersion of carbon nanotubes. Subsequently, the solution is cured after a hardener is added to form a hard state composite. Several means are followed to disperse particles in epoxy resins for making such composites like solution mixing and blending [5]. Such methods cannot produce major improvements in carbon nanotubes/epoxy composite due to lack of controlled orientation and ineffective dispersion of filler content in the epoxy resin matrix. Aligned carbon composites were successfully fabricated by hosting metallic magnetic particles upon the open edges of MWCNTs in order to bring, with the aid of a magnetic field, an out-of-plane arrangement of MWCNTs in a composite material. These unbroken and longitudinal carbon yarn can be assembled together to form a carbon nanotube/polymer composites [6]. Cortes et al. [7] and Bhamidipati [8] studied the tensile properties of nanofibers reinforced polymer matrices and showed only a slight increase in the tensile modulus and strength of the nanocomposites. They concluded that in order to significantly improve the mechanical performance of the nanocomposites, the nanotubes should exhibit a certain degree of alignment within the matrix phase. Barrera et al. [9] manufactured composites based on highly oriented nanotubes and nanofibers and observed a substantial improvement on their mechanical properties over non-oriented based nanocomposites.

The aim of the present work is to simulate the tensile stress-strain curves for composite materials reinforced with multi-wall CNTs arranged in in-plane and out-of-plane direction and develop a quantitative micromechanical model for the elastic properties of CNT-composites.

2. Theory

Eshelby problem is used to determine the stresses and strains distribution in the solid. A sufficient condition is to match both the elastic stress and the total strain field inside the transformed inhomogeneity and inside the equivalent inclusion. To replace inhomogeneity with an equivalent inclusion, both the traction force and the displacement field on the interface (S0) should be matched**.**

The stress strain fields inside the solid can be constructed by superimposing two sets of fields. First, that the solid containing the inhomogeneity is subjected to a uniform strain ε^A_{ij}, which is the strain throughout the solid under the applied load if the entire solid has elastic constant Cijkl**.** The stress field inside the matrix is σ^Aij = Cijkl ε^A_{kl}. While the stress field inside the in homogeneity is $\sigma^{A\wedge}$ij= C^ijkl ε^A_{kl} .The equilibrium condition would not be satisfied unless a body force $T_j = (\sigma^{A\wedge}_{ij} - \sigma^A_{ij})n_i$ is applied to the surface S_0 of the inhomogeneity.

Superimposing these two sets of fields, the elastic stress field inside the inhomogeneity is:

$$\sigma^I_{ij} = \mathrm{C}^{\wedge}_{\mathrm{ijkl}}\left(\varepsilon^A_{kl} + \varepsilon^{C'}_{kl}\right). \qquad (1)$$

Where $\varepsilon^{C'}_{kl}$ is the strain field at the interface due to the applied load $T_{j.}$

The total strain field inside the inhomogeneity is the same as its elastic strain:

$$\varepsilon_{ij}^{I} = \varepsilon_{ij}^{A} + \varepsilon_{ij}^{C'} . \tag{2}$$

The stiffness contribution tensor *N* of an inclusion is defined by the following:

$$\sigma_{ij} = C_{ijkl}^{o} \ \varepsilon_{kl} + N_{ijkl} \ \varepsilon_{kl} . \tag{3}$$

If all inclusions have identical shapes, and they have either random or uniform orientation, the general parameter, ∑*N*, can be expressed as a function of volume fraction by v_f and the shape factor by g:

$$N = v_f \left[\left(C^{*} - C^{o} \right)^{-1} + (P) \right]^{-1} \tag{4}$$

The Eshelby's solution has been carried out using Mori-Tanaka model. It is a mean-field homogenization based program. It uses Eshelby-based-analytical mean-field homogenization approaches and an analytical description of the material in order to compute the mechanical properties of a composite as a function of its microstructure morphology, i.e. inclusion geometry, orientation, volume fraction. It is found that the strain concentration tensor, B^{ε}, relating the volume average strain of all inclusions to the matrix strain, as given by:

$$B^{\varepsilon} = H^{\varepsilon}(I, C_o, C_1). \tag{5}$$

This is exactly the strain concentration tensor of the Eshelby's single inclusion problem. The M-T model is very successful in predicting the effective properties of two-phase composites. Each inclusion in the real RVE behaves as if it were isolated in the real matrix. The body is infinite and subjected to the average matrix strains in the real RVE as the far field (remote) strain. The macroscopic stiffness is given as:

$$C = C_o + N_{NI} : \left[(1 - f)(C^{*} - C^{o}) + N_{NI} \right]^{-1} : (C^{*} - C^{o}). \tag{6}$$

3. Results

The microstructure is created by defining the constituent phases; each one should follow a prescribed material model. Elastoplastic with exponential law is defined as a constitutive material model for the resin material (Epoxy). Dimensions of approximately 40nm diameter and 15µm lengths were defined into the model. After the microstructure has been created, the RVE is subjected to a uniformly 0.05 axial strain. Macroscopic stress strain data were post processed after the solution is complete. Predicted properties of the composites are compared with those obtained using a Universal Instron machine under quasi-static loading at room temperature [6]. Results for in-plane Young's modulus of the composite reinforced with nanotubes randomly oriented are also presented in Fig 1.

Stiffness property for composite in which CNT were aligned through thickness direction is presented. The modulus of elasticity for the through thickness aligned composites remains almost unaltered much by increasing the nanotubes volume fraction. Comparison of the experimental measurements of out of plane Young's modulus with Micro-mechanical prediction is given in Fig 2. On the other hand, Stiffness results for in-plane CNT composite in which CNT were randomly oriented are presented in Fig 3. When examining the stress-strain curves, no yield point has been noticed over the entire deformation loading. Unlike the aligned fiber system, modulus of elasticity for randomly dispersed system increase much with increasing the nanotubes volume fraction. However, Discrepancy between predicted stiffness and the tested ones is prominent. These differences become more when we go for higher loading of reinforcements as it is the case for 46%. The poor correlation between the model and experiments is argued to be most likely a result of variations in the size of the nanotubes used which is taken fixed in the model.

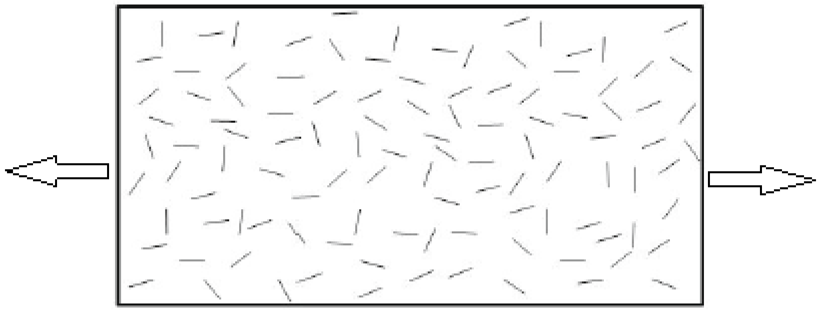

Fig 1. Schematic showing in-plane fibers with randomly orientation.

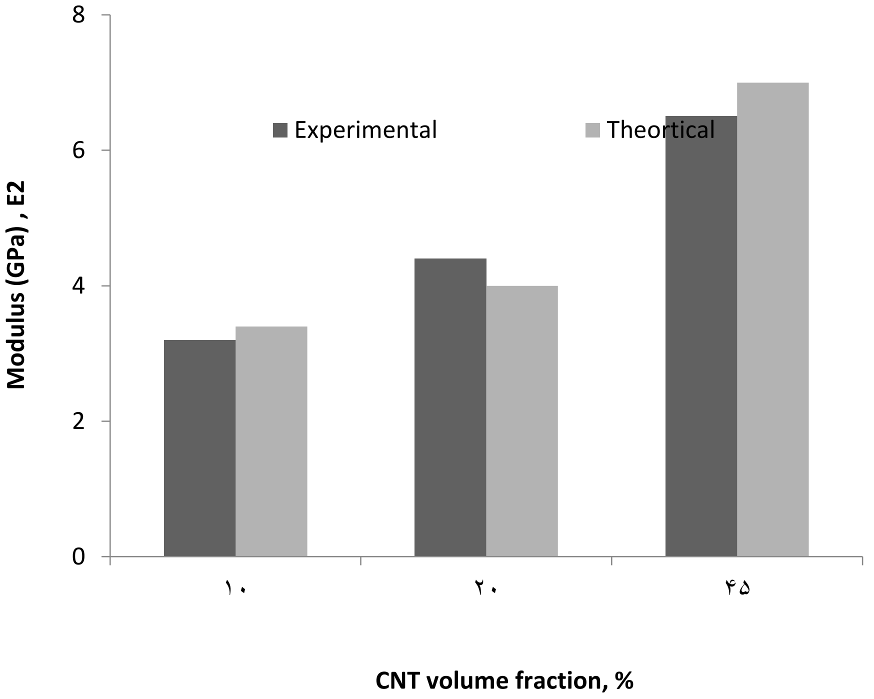

Fig 2. Comparison of the experimental measurements of out-plane Young’s modulus with micromechanical prediction for aligned CNT composites.

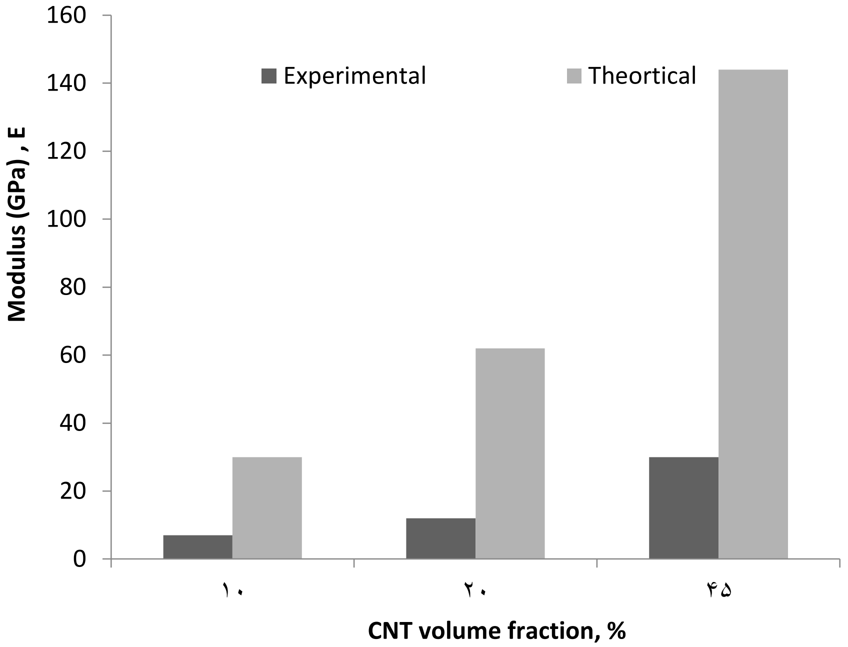

Fig 3. Comparison of the experimental measurements of in-plane Young's modulus with micromechanical predictions for randomly dispersed CNT composites.

4. Conclusions

Aligned carbon nanocomposites have been successfully manufactured by introducing metallic magnetic particles upon the open edges of MWCNTs [6]. It allows one to control the nanotubes orientation in the composite. Tensile properties of Multi-Wall Carbon Nanotubes (MWCNT) reinforced polymer matrix composites with nanotubes aligned in out-of-plane direction and randomly in-plan orientation have been theoretically investigated. Both experimental measurements [6] and micromechanical modeling are addressed. The modulus of elasticity for the through thickness aligned composites remains almost unaltered much by increasing the nanotubes volume fraction. However, stiffness property for randomly dispersed system increases much with increasing the nanotubes volume fraction. Poor correlation between predicted stiffness and the tested one was observed for those composites with randomly in-plane fiber structure. Discrepancy becomes more prominent with increasing filler content inside the composite.

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