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Investigating the mechanical properties of single walled carbon nanotube reinforced epoxy composite through finite element modelling

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ABSTRACT

Varying experimental results on the mechanical properties of carbon nanotube reinforced polymer composites (CNTRPs) have been reported due to the complexities associated with the characterization of material properties in nano-scale. Insight into the issues associated with CNTRPs may be brought through computational techniques time- and cost-effectively. In this study, finite element models are generated in which single walled carbon nanotube models are embedded into the epoxy resin. For modelling interface regions, two approaches named as non-bonded interactions and perfect bonding model are utilized and compared against each other. Representative volume finite element (RVE) models are built for a range of CNTRPs and employed for the evaluation of effects of diameter and chirality on the Young's modulus and Poisson's ratio of CNTRPs, for which there is a paucity in the literature. The outcomes of this study are in good agreement with those reported available in the literature earlier. The proposed modelling approach presents a valuable tool for determining other material properties of CNTRPs.

1. Introduction

1.1. Overview

Researchers in both industry and academia are taking a keen interest in developing advanced nanocomposites with multifunctional features. Carbon nanotubes (CNTs) are unique nanostructured materials which possess extraordinary physical and mechanical properties. It is their remarkable properties that bring interest in using CNTs as filler in polymeric matrix to get ultra-light structural materials, which are referred to as carbon nanotube reinforced polymer composites (CNTRPs) [1]. Diverse experimental results on the mechanical properties of CNTRPs have been reported by various researchers and scientists since their emergence, some of which are discussed as follows to explain the necessity of further research in this highly competitive area.

When CNTs with their unparalleled high elastic modulus and tensile strength are integrated into a polymer matrix, it does not always ensure enhancement in mechanical properties of the composite. Both encouraging and discouraging results have been seen in the past. In some studies, mechanical properties even degraded when CNTs were added to a polymer matrix. Bhattacharya et al. [2] investigated melt blended composite of single walled carbon nanotube (SWNT)/PP (polypropylene) and observed a minute drop in elastic modulus, tensile strength and fracture strain with 0.8 wt.% CNT addition. In another research conducted by Lau and Shi [3], flexural strength of CNT/epoxy composite failed to increase with 2 wt.% CNT addition. Jia et al. [4] determined that tensile strength, hardness and toughness of the CNT/PMMA (poly methyl methacrylate) composite decreases with untreated CNT.

Some studies exhibit slight increase in elastic modulus with almost no increase in mechanical strength of CNTRPs. Schadler et al. [5] presented in their study that the tensile elastic modulus of CNT/epoxy composite was improved by about 20% while 24% improvement was made in the compressive elastic modulus by adding 5 wt.% of CNT into the polymer matrix. In a study by Haggenmueller et al. [6] on aligned SWNT/PMMA composite, elastic modulus and yield strength were reported to increase moderately with an increase in draw ratio and nanotube loading. Wong et al. [7] studied multi walled carbon nanotube (MWNT)/PS (polystyrene) rod samples from an extrusion process. They observed that tensile stiffness was increased by approximately 10% and tensile strength was also somewhat improved.

In some cases, the mechanical properties were improved significantly by the reinforcement of CNTs into polymer matrices. A

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study by Qian et al. [8] showed that both elastic modulus and tensile strength of MWNT/PS composite was increased by 36–40% and 25%, respectively, after adding 1 wt.% CNT into the matrix. Liu et al. [9] compared the elastic modulus and yield strength of neat PA6 (nylon-6) and MWNT/PA6 composite and their results showed that by incorporating only 2 wt.% MWNT, modulus and strength enhanced by about 214% and 162%, respectively, for the composite. Ganguli et al. [10] demonstrated that with the addition of 1 wt.% of MWNT in the polymer matrix of a bi-functional epoxy resin, ultimate strength and strain to failure improved up to 139% and 158%, respectively.

A large number of experimental studies have been carried out to estimate the mechanical properties of CNTRPs and the above literature review suggests that there exists a variability among these experimental results due to the complexities mainly associated with the characterization of material properties in nano-scale [11]. Also, there is a paucity in the literature on the effects of size and chirality on the mechanical properties of CNTRPs. Insight into the aforementioned issues may be brought through computational techniques time- and cost-effectively as compared to experimentation. Computational modelling of CNTRPs for the assessment of their mechanical properties is thought to be a powerful tool when compared to the experimental handicaps. This creates an opportunity to investigate CNTRPs more in detail.

1.2. Modelling of CNTRPs

SWNT is considered by most of the researchers to be one of the ultimate reinforcements for the next generation high performance composite materials. MWNT possesses lower mechanical, electrical and thermal properties due to the fact that the concentric nanotubes slide past each other under axial tensile loading [12]. Hence, SWNTs are studied as reinforcements for CNTRPs in this study. A few studies are found in literature on modelling of CNTRPs by embedding SWNTs into the polymer matrix. In order to study the effect of CNT on fracture properties of the polymer composite, Rafiee et al. [13] constructed a 3D finite element model of single-walled carbon nanotube reinforced polymer. The representative volume element (RVE) took into account the lattice structure of CNTs and simulated the surrounding polymer using solid elements. They used van der Waals interactions for load transfer from the host polymer matrix to the CNT. In the next step, they replaced CNT and interface region by perfectly bonded solid fibre with Young's modulus of 1 TPa for investigating the importance of lattice structure of CNT and non-bonded interface region in modelling process. They concluded by claiming that non-bonded interface region is a better approach for reinforcement against crack propagation.

Rafiee and Moghadam [14] investigated the impact and post-impact behaviour of a CNTRP based on cylindrical representative volume element (RVE) consisting of SWNT dispersed into a polymer matrix. A 3D beam element was used to model each C–C bond in the CNT lattice structure. CNT and polymer matrix were simulated at nano and micro scale respectively. The interface region between CNT and polymer matrix was modelled using van der Waals forces. These van der Waals forces and the nodes of the inner surface of the matrix were modelled using 3D non-linear spring elements whose properties were defined by Lennard-Jones (L-J) potential. Simulations were also performed for the neat polymer resin RVE, i.e. not reinforced with CNT. Axial impact loading was applied at one end of the cylinder while zero displacement boundary conditions were imposed at the other end. Their simulations demonstrated that the maximum axial deflection was six times greater for the neat resin as compared to CNTRP. Also, the maximum tensile stress at the fixed end was found to be higher for the neat resin. Therefore, they concluded that even a small fraction of 5% by volume of CNTs improves the impact resistance of the polymer matrix.

Odegard et al. [15] assumed perfect covalent bonding between CNT and polymer resin in the presence of poly m-phenylenevinylene (PmPV) oligomers. Shokrieh and Rafiee [16] modelled armchair RVE using equivalent-continuum approach and compared their model with Odegard et al. [15]. They considered van der Waals interactions between the two phases and in order to predict the mechanical behaviour of the CNT/polymer composites, they used equivalent long fibre in place of a straight CNT embedded into a polymer matrix with van der Waals interface region. They found highly non-linear behaviour of their constructed model under tensile loading. They also determined the mechanical properties of the equivalent long fibre consisting of CNT and its interface region.

Ayatollahi et al. [17] proposed a multi-scale RVE representing CNTRP for finding the mechanical behaviour under tensile, bending and torsional loading of the nanocomposites. They found the effect of interface stiffness on tensile, bending and torsional properties on two RVE configurations. The stiffness of the RVE was found to be affected much more by a strong interface than by a weaker interface with a low value of Young's modulus. Furthermore, the stiffness of the nanocomposite was found to be most affected by the stiffness of the interface under bending loading conditions.

Karimzadeh et al. [18] modelled both cylindrical and square RVEs to evaluate the effective mechanical properties of CNT-based composites. They developed a formulation based on 3D elasticity theory. For the estimation of Young's modulus in the axial direction of the RVE and validation of the numerical solutions, an extended rule of mixtures was derived. They found that the modulus of elasticity can be increased 10 times with only 5% of nanotube reinforcement. For further research they highlighted that large simulation models for CNT based composites should be developed, which can link nano, micro and macro scale models together.

1.3. Aims and objectives

This study mainly presents modelling of carbon nanotube reinforced polymer composites (CNTRPs) by using finite element technique. The primary objective of this work is to determine the effect of SWNT chirality and diameter on the Young's modulus and Poisson's ratio of the SWNT/epoxy composite, for which there is a paucity in the literature. For this purpose, the equivalent beam element model is introduced for SWNTs and is employed to build SWNT/epoxy composite signified by a cylindrical representative volume element (RVE). Also, different approaches in modelling these cylindrical RVEs are compared against each other and validated by utilizing both the values published in literature and the theoretical relation called 'continuum rule of mixtures'. The comparison itself is considered to be a contribution since the van der Waals approach is developed recently and has not been sufficiently studied.

2. Modelling representative volume element (RVE)

2.1. RVE geometry

The RVEs are predominantly classified into three in the form of circular, square and hexagonal cross-sections in the literature in order to model CNT based composites [18,19]. These classifications are based on the shape of their cross-section as shown in Fig. 1. These RVEs are essential to provide detailed analyses of SWNTs interacting with the polymer matrix such as mechanisms for load transfer, stress distributions, and adhesion of the two phases.