REINFORCEMENT EFFICIENCY OF CARBON NANOTUBES: PROBABLISTIC STUDY OF NANOTUBE WAVINESS

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Introduction

Carbon nanotubes are received huge interest as the reinforcing agents of polymeric composites due to their high exceptional mechanical properties [1]. Prediction of CNT/polymer composites properties plays an important role in their development process. CNT is a reinforcing agent at nano-scale; however, mechanical properties of CNTRP are subjected to be characterized at macro-scale. The diversity of involved scales (Nano, Micro, Meso and Macro) demands a proper multi-scale modeling approach. On the other side, there are some process-induced uncertainties in CNTRP which should be taken into account in the simulation process. Length, orientation, agglomeration, dispersion and curvature of CNTs are most important non-deterministic parameters.
The main goal of this research is to study the influence of wavy CNTs on elastic properties of CNTRP.

Simulation outline

As the first phase of simulation procedure, a top-down scanning is performed to identify the effective parameters of each specific scale. It is found that the waviness of CNT should be taken into account at the scale of meso. Then, *N3M* multi-scale modeling technique is employed to predict the Young's modulus and Poisson's Ratio of CNTRP. The utilized multi-scale model starts simulation from the scale of nano and will last in macro scale passing the in-between scales of micro and meso. Different involved length scales are schematically depicted in Fig. 1 on the basis of top-down scanning method. Due to different levels associated with the material region, it is necessary to identify effective parameters of each and every scale. Subsequently, suitable representative volume element (RVE) should be defined for each scale separately to simulate corresponding effective parameters, accordingly. The involved parameters categorized by effective scales are presented in Table 1.
At nano-scale each Carbon-Carbon (C-C) bond was replaced with beam element and the lattice molecular structure was substituted with an equivalent discrete frame structure [2]. For this purpose a linkage developed by Li and Chou [3] between molecular mechanics and structural mechanics was used.

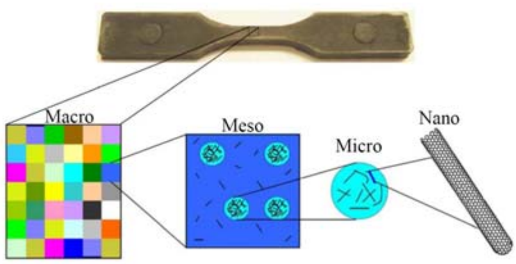

Fig. 1: Involved scales in simulation of CNTRP

At micro scale, a multi-scale finite element model of the carbon nanotube, non-bonded interphase region and surrounding polymer was constructed [4]. Carbon nanotube and the interphase region were converted to an equivalent fiber [5].

Table 1: Effective parameters for each scale of simulation

Scale	Parameters
Nano	Molecular interactions, bond configurations, CNT diameter& chirality
Micro	Interaction between CNT and polymer, Stress transfer in interphase, CNT length
Meso	Volume fraction, orientation of CNT, Agglomeration, Dispersion, CNT curvature
Macro	Non-uniform distribution of inclusions

The RVE of the meso-scale is presented in Fig. 1. Following to the developed method of simulation at very lower scale of micro, the RVE at meso-scale consists of developed equivalent fiber instead of a CNT. Using equivalent fiber technique, micromechanics equations will be applied to CNTRP indirectly. Embedded equivalent fibers in presented block of Fig. 1 are oriented in random directions and they can exist in both of straight and curved configurations. They can be either concentrated in local aggregates or dispersed in some other areas. It is assumed that aggregates will appear in the form of spherical regions. All other equivalent fibers located out of the spherical regions are considered to be fully dispersed. Young's modulus and Poisson's ratio of the constitutive blocks can be calculated using improved model of Shi, et al. [6].

The effect of nanotube waviness as an effective parameter of meso-scale is considered on the basis of developed bounding technique accounting for properties of developed equivalent fiber at micro scales. Due to the random shapes of wavy carbon nanotubes, stochastic study is performed to simulate any arbitrary shape of non-straight CNTs.

The material region at macro scale is partitioned into different constitutive blocks with different properties. This portioning strategy simulates material in-homogeneity caused by uncertainties in manufacturing process of CNTRP. The properties of each constitutive block are calculated on the basis of modeling process at meso-scale. The overall properties of investigated material region can be calculated using averaging method on the properties of each and every block.

The results reveal that non-straight carbon nanotubes play an important and significant role in reducing reinforcement efficiency of carbon nanotubes. It is observed that Young's modulus of wavy CNT/polymer decreases 18% in comparison with straight CNT/polymer when the volume fraction of CNT is 5%; while Poisson's ratio increases 2.5%. Fig.2 shows the effect of CNT waviness on stiffness reduction of carbon nanotube reinforced polymer.

Conclusions

A full stochastic multi-scale modeling approach is developed to predict Young's modulus and Poisson's ratio of CNTRP. The influence of CNT waviness on overall properties of CNTRP has been studied. It was revealed that results are highly sensitive to the curvatures of the CNTs.

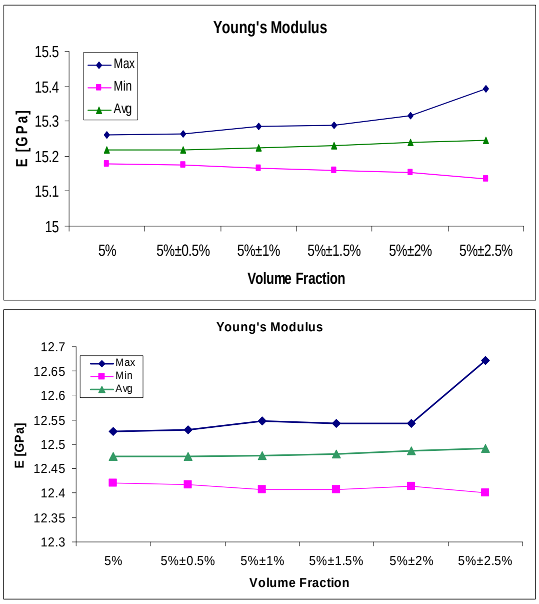

Fig. 2: Young's modulus of CNTRP with straight CNT (top) and non-straight CNT (bottom)

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