DEVELOPMENT OF A STOCHASTIC SIMULATION TO PREDICT ELASTIC PROPERTIES OF CARBON NANOTUBE REINFORCED COMPOSITES

Mahmood M. Shokrieh, R. Rafiee

Composites research laboratory, Center of Excellence in Experimental Solid Mechanics and Dynamics, Mechanical Engineering Department, Iran university of science and technology, e-mail: shokrieh@iust.ac.ir, rafiee@iust.ac.ir

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Summary. The main objective of this research is to predict Young’s modulus and Poisson’s ratio of carbon nanotube reinforced polymer (CNTRP). A full stochastic multi-scale modeling technique is developed to consider all affected parameters of all nano, micro, meso and macro-scales. The length, orientation, agglomeration, curvature and dispersion of the CNTs are taken into account as random parameters. Comparing results of simulation with experimental observations, it is shown that developed method is an efficient tool to predict elastic properties of CNTRP.

1 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 micro-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. Therefore, stochastic implementation of simulation to accounts for random parameters is necessary. In this research, a full range multi-scale model is developed to predict elastic properties of CNTRP.

2 SIMULATION OUTLINE

A hierarchical multi-scale modeling is developed to simulate CNTRP. Since the developed technique will cover all scales of nano, micro, meso and macro, it will be referred to hereinafter as “N3M” multi-scale modeling. Different stages of proposed modeling procedure at each scale will be constructed on the basis of bottom-up modeling approach. 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.

<table>
<thead>
<tr>
<th>Scale</th>
<th>Length</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nano</td>
<td>nm</td>
<td>Molecular interactions, bond configurations, CNT diameter, CNT chirality</td>
</tr>
<tr>
<td>Micro</td>
<td>nm/μm</td>
<td>Interaction between CNT and polymer, Stress transfer in interphase, CNT length</td>
</tr>
<tr>
<td>Meso</td>
<td>μm</td>
<td>Volume fraction, orientation of CNT, Agglomeration, Dispersion, CNT curvature</td>
</tr>
<tr>
<td>Macro</td>
<td>mm</td>
<td>Non-uniform distribution of inclusions, mechanical properties</td>
</tr>
</tbody>
</table>

Table 1: Effective parameters for each scale of simulation

The flowchart of developed multi-scale modeling is presented in Fig. 2. 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. 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].

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. So, it is permissible to utilize micromechanics equations at meso-scale. Using equivalent fiber technique, micromechanics equations will be applied to CNTRP indirectly. Embedded equivalent fibers in presented block of Fig. 1 are oriented in

![Figure 1: Involved scales in simulation of CNTRP](image)
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. As shown in Fig. 2, Young’s modulus and Poisson’s ratio of the constitutive blocks can be calculated using improved micromechanics model of Shi, et al. [6].

Figure 2: Flowchart of developed stochastic $N3M$ multi-scale modeling

As it is illustrated in Fig. 1, the material region at macro scale is partitioned into different constitutive blocks with different properties. This partitioning strategy simulates material inhomogeneity 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 and will be used here as input data. The overall properties of investigated material region can be calculated using averaging method on the properties of each and every block.

3 CONCLUSIONS

A full stochastic multi-scale modeling approach is developed to predict Young’s modulus and Poisson’s ratio of CNTRP. The novelty of the current research is development a full-range multi-scale technique to consider effective parameters of all nano, micro, meso and macro-scales and full stochastic implementation of integrated modeling procedures. The length, orientation, agglomeration, curvature and dispersion of the carbon nanotubes are taken into account as random parameters. It is proven that random distribution of carbon nanotube length and volume fraction can be replaced with corresponding mean values. The results of predictions are in a very good agreement with published experimental observations.

REFERENCES