HIERARCHICHAL MULTI-SCALE MODELING OF CNT-COATED FIBER-REINFROCED LAMINATES

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1. Introduction

Due to the supreme mechanical properties of carbon nanotubes (CNTs) [1] from one hand, and difficulties of CNT dispersion in polymer from the other hand; a new category of fiber has been recently developed known as “fuzzy fiber”. A terminology of “fuzzy fiber” indicates a core micro-fiber where CNTs are grown on its surface. The CNT coated fiber is impregnated with the resin forming fuzzy fiber reinforced polymers [2-4]. The core fiber which plays the role of primary reinforcement can be appeared in the form glass, ceramic or carbon fibers. The CNTs grown on the surface of core fiber can be viewed as the secondary reinforcement in fuzzy fiber reinforced laminates. Reinforcing a polymer matrix with fuzzy fibers not only enhance the fiber/matrix interphase properties in comparison with using untreated micro-fibers [5]; but also improve matrix-dominated properties in the composites because of improved load transferring from the matrix to treated fibers. Thus, the advantage of incorporating fuzzy fiber into matrix is twofold: (i) improvement in the fiber-matrix bonding quality and; (ii) overcoming the main shortcoming of Uni-Directional fiber reinforced composites recognized as low mechanical properties in the transverse direction to the fiber. The main goal of this article is to develop a multi-scale modeling approach to predict mechanical properties of fuzzy fiber reinforced laminates starting from the scale of nano and ending to the macro scale, passing in-between scales of micro and meso. Thus, a bottom-up modeling procedure is developed taking into account CNT at the nano-scale while the properties of fuzzy fiber reinforced laminated are characterized at the macro-scale.

2. Framework of multi-scale modeling

Hierarchical multi-scale modeling is developed for the purpose of this study wherein the output of simulation at each scale is fed to the very upper scale as the input data. In this strategy, the interphase layer between core fiber and surrounding polymer is taken into account as a distinct phase comprises of CNT reinforced polymers. Different scales of modeling are depicted in Fig. 1.

At the scale of nano, lattice structure of CNT is modeled in commercial FE package. Each C-C bond is replaced with an equivalent beam element. The properties of the beam element are obtained by establishing a correlation between the interatomic potential energy of molecular space with strain energy of structural mechanic space. At the scale of micro, the interaction between CNT and surrounding polymer is modeled using non-linear spring elements representing van der Waals interactions. Performing a FE analysis, CNT and its surrounding interphase is replaced with a virtual equivalent fiber as a continuum medium. While the Young’s modulus of isolated CNT is estimated at nano-scale about 1 TPa, the longitudinal Young’s modulus of the equivalent fiber is obtained about 649 GPa. Transverse Young’s modulus, Poisson’s ratio and in-plane shear modulus of the equivalent fiber is obtained as 11.27 GPa, 0.284 and 5.13 GPa, respectively. The obtained properties imply on the transversely-isotropic behavior of the equivalent fiber. At the scale of meso, the properties of the CNT/polymer nanocomposites around core fiber is obtained using Mori-

Tanaka formulations [6] and it is combined with the mechanical properties of the core fiber using concentric cylinder technique [6]. After obtaining the properties of a single fuzzy fiber, Halpin-Tsai [6] micromechanics rules are employed to predict mechanical properties of the fuzzy fiber reinforced laminated. The whole explained procedure is executed stochastically, treating CNT curvature shape and volume fraction as random parameters. In each realization, CNT volume fraction is chosen randomly in complete accordance with overall CNT volume fraction. Moreover, the longitudinal and transverse moduli of the equivalent fiber are randomly and independently chosen between 649 and 11 GPa capturing arbitrary shape of CNT. The procedure is executed 1500 times to generate sufficient random samples for the purpose of stochastic modeling.

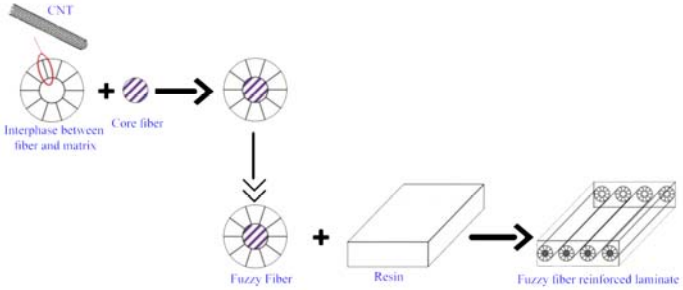

Fig. 1: Bottom-up modeling of fuzzy fiber reinforced laminate

4. Results and discussion

Developed modeling is implemented to simulate the specific case study performed by Kulkarni et al. [4] through the experimental observations. It is revealed that performing a deterministic calculation, the transverse modulus of the fuzzy fiber reinforced laminate is obtained as 11.2 GPa. While the stochastic modeling achieves 10.00 GPa which is in a very good agreement with measured10.2 GPa for the same mechanical property. This implies on the importance of taking into account random variables during the simulation procedure. A parametric study is also conducted to examine the degree to which CNT volume fraction will improve the transverse modulus of a single fuzzy fiber.

6. References

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