Multiscale Modeling of Carbon Nanotube-based Nanocomposites using Computational Mechanics Approach

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Abstract

Carbon nanotubes (CNT) possess novel properties that make them potentially useful in many applications, which take full advantage of its unique properties of aspect ratio, mechanical strength, electrical and thermal conductivity. Techniques have been developed to produce nanotubes in sizeable quantities, including arc discharge, dual-phase laser, chemical vapor deposition, ball milling, low-temperature solid pyrolysis, flame synthesis etc. However, the properties and characteristics of CNTs and CNT based nanocomposite are still being researched heavily to explore the potentials of these emerging composites. Recent studies have proven what these nanocomposite can offer to a wide spectrum of applications. This research work is aimed to investigate the mechanical behavior of a single graphene sheet, a single wall carbon nanotube (SWCNT), and a single wall carbon nanotube embedded in a polymer at nano-level, and scaling it up to micro-level to obtain a realistic estimation of its mechanical properties.

Atomistic-based continuum model is developed to determine the Young’s and shear moduli and the Poisson’s ratio of two types of nano-reinforcements i.e. SWCNT and graphene layer. The stored energy in a representative unit cell of nano-reinforcements at atomistic scale was equated to the strain energy of an equivalent continuum medium under prescribed boundary conditions. These displacement-controlled (essential) boundary conditions, which generate a uniform strain field in the unit cell model were used to calculate one elastic modulus at a time. Three to five atomistic finite element models were adopted with an assumption that force interactions among carbon atoms can be modeled by either spring or beam elements. The elastic moduli of nano-reinforcements are determined based on the proposed modeling approach, which allowed to calculate effective Young’s and shear moduli and Poisson’s ratio. The results were found in a good agreement with the published theoretical and numerical data. However, Poisson’s ratio exhibits sensitivity to the considered atomistic model. This observation is supported by a significant variation in estimates as can also be confirmed by published results.