Influence of Manufacturing Defects on the Nanostructure-Mechanical Property Relationships in CNT-Reinforced Nanocomposites

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Abstract:

Carbon nanotubes are increasingly being used as reinforcements in polymer composite materials, in aerospace, mechanical, and automotive industries. However, an adequate understanding of their nanostructure-mechanical property relationships is still lacking. In practical industrial manufacturing, random defects and imperfections are unavoidable. These have significant influences on such relationships. In the present study, these influences are investigated. Carbon-Nanotube-Reinforced-Polymer Composite material containing structural vacancy defects in the nanotubes is considered. Computational material modeling approach is followed since experimental investigations are not feasible. A multiscale finite element model of a Representative Volume Element of the nanomaterial is developed to characterize the material properties of the nanocomposite material. The multiscale material model comprises a Single-Walled Carbon Nanotube, an interface, and a polymer matrix. The SWCNT is treated as a space nano-frame characterized by the modified Morse potential, while the polymer matrix is characterized using the Mooney-Rivlin strain energy. The interface is characterized using van der Waals links based on the Lennard-Jones potential. The Monte Carlo Simulation methodology is used to represent vacancy defects in the nanotube and corresponding van der Waals links. Mechanical properties of the nanocomposite material are predicted and the nanostructure-mechanical property relationships are characterized. Practical aspects in nanomaterial development are synthesized.