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On the Modeling CNT-Polymer Interaction Using Different Approaches

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Naturally, Carbon Nanotube (CNT) interacts with surrounding polymer through weakly non-bonded van der Waals (vdW) interactions. Since the basic assumption of perfect bonding between reinforcing agent and surrounding polymer is not valid at the scale of nano, direct application of micromechanical rules for predicting mechanical properties of CNT reinforced polymer is not permissible. Those micromechanical rules taking into account three separate phases for reinforcing agent, intermediate phase and matrix cannot be either used, since mechanical properties of the intermediate region between CNT and polymer are not characterized experimentally. Moreover, no material region exists between CNT and polymer and the space include molecular interactions.
Three different approaches consisting of atomistic modeling, semi-continuum modeling and continuum modeling are employed to investigate the mechanical properties of an embedded CNT in polymer. Thus, a micro-scale RVE containing CNT, polymer and CNT-polymer interaction is constructed and analyzed. Then, CNT and CNT-polymer interaction are integrated into a virtual continuum medium called equivalent fiber and the mechanical properties of equivalent fiber are obtained. A comparative study is performed between computed results through different methods. The results reveal that mechanical properties of the equivalent fiber is considerably less than an isolated CNT due to the influence of CNT-polymer interaction and also all three approaches address close values implying on independency of results to the employed technique of simulation.

Keywords: Carbon nanotube; Non-bonded interaction; Molecular Dynamics Simulation; Continuum modeling; Semi-continuum Modeling