Abstract

Carbon fiber reinforced plastic (CFRP) composites are widely used in the aerospace industry for enhanced thermo-mechanical properties. Most of these structures comprise thermoset polymer matrices and carbon fibers. Nano-fillers as secondary reinforcements have the advantage of enhancing mechanical, thermal and electrical properties of the matrix. There is a lack of consensus in estimation of the degree of enhancement due to nano-reinforcements. Therefore, the present work focuses on analyzing the inherent mechanical and thermal properties of nano-composites with fillers. Atomistic modeling, i.e., molecular dynamics (MD) is chosen for the detailed extraction of properties which are prone to uncertainties from physical experiments. Carbon networked (sp^2) one dimensional and two dimensional nano-structures of carbon nanotube (CNT) and graphene are selected as primary fillers for thermoset polymers. The MD simulations have been carried out using adaptive intermolecular reactive empirical bond order (AIREBO) potential with cut-off function parameters $1.42\mathring{A}$ and $2.46\mathring{A}$ to avoid non-physical behaviors. The hexagonal networked carbon structures are defined by a parameter called chiral angle. The changes in the angle show significant impact on material and geometrical properties. The diameter of a CNT has been chosen and CNTs with various available topologies have been generated by changing the chiral indices keeping the diameter fixed. Graphene structures with chiral indices equivalent to those of CNT structures have been considered. The uniaxial tensile tests have been performed on all the structures using MD simulations. The dependency of ultimate stress, ultimate strain, Young's modulus, fracture stress, fracture strain and Poisson's ratio on chirality of the structures has been investigated. The thermoset polymer consists of the epoxy, Di- glycidyl ether of Bisphenol-F (DGEBF) monomer, and the hardener, Di-ethylene Toluene Diamine (DETDA). The epoxy is commercially known as EPON 862. The static cross-linking at a ratio of 4:1 has been adopted to model the representative cross-linked polymer (RCP) of EPON862. The nano-fillers are chosen under various considerations like SWCNT, CNT Bundle, graphene Sheet, and graphene layers. The CNT and CNT Bundle nano-fillers are designed with end caps, which enhance the mode I (opening mode) fracture toughness. The MD simulations of nano-composites have been carried out with various weight fractions of epoxy and nano-fillers. All the studies have been conducted in an amorphous structure that contains nano-fillers reinforced with cross-linked epoxy. The soft experiments of models are conducted under tensile test conditions along different principal axes. The stress-strain behavior of the amorphous cell has been interpreted in this work. The nano-composites have been analyzed with various lengths and diameters of nano-fillers to study the effect of aspect ratio on interfacial strength. The amount of epoxy content has been balanced with the corresponding uniform increase in weight fraction. The energy release rate for creation of new fracture surface has been computed from simulations. In addition, the details of crack surface area have been obtained through the post-processing of iso-surfaces. The fracture toughness has been analyzed for different types of nano-filler reinforced thermoset polymers.

Keywords: Nano-composites, molecular dynamics, carbon nanotube, graphene, thermoset polymer.