INTERFACIAL AND MECHANICAL STUDIES ON AMINE FUNCTIONALIZED CARBON NANOTUBES IN EPOXY COMPOSITE THROUGH AB-INITIO AND MOLECULAR DYNAMICS SIMULATIONS

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ABSTRACT

CNT-epoxy nanocomposites owing to their superior thermo-mechanical properties have attained a great deal of attention since the end of last decade. Modelling such nanocomposites with realistic desnities remains a non-trivial issue in Molecular Dynamics (MD) because of their inherently irregular cross-linked networks. In this report a new approach for modelling functionalized-CNT reinforced epoxy polymer network is presented. A coarse-grained melt of discrete DGEBA monomers, ethylene diamine (curing agent) and amide functionalized CNTs is made to form C-N cross-links under pressure. The resulting network is reverse mapped onto its fine-grained structure and relaxed by use of cyclic NPT/NVT runs. Increased diffusional motion and reduced steric hindrance offered by the coarse-grained model avoids atomic overlaps and facilitates swift relaxation of the instabilities introduced due to cross-linking.

The next portion of the report deals with mechanical and fracture properties of the CNT-epoxy nano-composite. Fracture study on polymer networks also pose a challenge in MD owing to the availability of only approximate MD potentials for organic molecules which are incapable of capturing bond failure/creation. In this work a modification to the existing pcff potential is made by incorporating failure bond lengths data from ab-initio (DFTB) calculations thereby enabling it to update the bond topology of the fine grained network at large displacements. The failure bond lengths are obtained by subjecting a small representative unit of the CNT-epoxy nanocomposite to an iterative straining scheme so as to identify the critical interfaces and their failure bond lengths. Elastic constants and fracture strength of the fine-grained CNT epoxy network are determined from MD/MM based straining experiments. A ~75% improvement in stiffness and ~33% increment in fracture strength is observed for the functionalized CNT-epoxy nanocomposite when compared to that of pure epoxy.

Keywords: ab initio, molecular dynamics, epoxy polymer, carbon nanotubes, functionalized, cross linking, coarse grained, fine graining, interfacial properties, strength, stiffness