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Comparison of epoxy matrices

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Multiscale Modeling of Carbon Fiber/Carbon Nanotube/Epoxy

Hybrid Composites: Comparison of Epoxy Matrices

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Abstract

This study addresses the multiscale modeling of hybrid composites composed of carbon fibers (CFs), carbon nanotubes (CNTs), and three different epoxy systems (di-, tri-, and tetra-functional resin epoxies). Molecular dynamics (MD) simulations are performed to predict the molecular-level interfacial and mechanical behavior of CNT embedded in epoxy. Micromechanics calculations are implemented to translate the molecular phenomena observed to predict the mechanical properties of CNT/epoxy composites with randomly oriented CNTs and CF/CNT/epoxy systems with aligned CFs and randomly oriented CNTs. The model is validated with experimental Young's modulus values for CNT/epoxy available in the literature. The results demonstrate that the tri- and tetra-functional resin epoxies demonstrate comparably high moduli over the di-functional resin for CNT concentrations up to 5 wt%. For higher CNT loadings, the tri-functional resin epoxy is predicted to outperform the other resins with respect to stiffness due to its strong interaction with CNTs and high bulk stiffness.

Keywords: A. Nano composites, Molecular dynamics, B. Mechanical properties, B. Interface,

B. Interphase

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