Accepted Manuscript

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PII: S0266-3538(17)32279-0

DOI: 10.1016/j.compscitech.2018.03.006

Reference: CSTE 7124

To appear in: *Composites Science and Technology*

Received Date: 11 September 2017

Revised Date: 25 February 2018

Accepted Date: 5 March 2018

Please cite this article as: Radue MS, Odegard GM, Multiscale modeling of carbon fiber/carbon nanotube/epoxy hybrid composites: Comparison of epoxy matrices, *Composites Science and Technology* (2018), doi: 10.1016/j.compscitech.2018.03.006.

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