Accepted Manuscript

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PII: S0266-3538(17)32618-0

DOI: 10.1016/j.compscitech.2018.02.008

Reference: CSTE 7084

To appear in: *Composites Science and Technology*

Received Date: 20 October 2017

Revised Date: 2 February 2018

Accepted Date: 7 February 2018

Please cite this article as: Jensen BD, Odegard GM, Kim J-W, Sauti G, Siochi EJ, Wise KE, Simulating the effects of carbon nanotube continuity and interfacial bonding on composite strength and stiffness, *Composites Science and Technology* (2018), doi: 10.1016/j.compscitech.2018.02.008.

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ABSTRACT

Molecular dynamics simulations of carbon nanotube (CNT) composites, in which the CNTs are continuous across the periodic boundary, overestimate the experimentally measured mechanical properties of CNT composites along the fiber direction. Since the CNTs in these composites are much shorter than the composite dimensions, load must be transferred either directly between CNTs or through the matrix, a mechanism that is absent in simulations of effectively continuous CNTs. In this study, the elastic and fracture properties of high volume fraction discontinuous carbon nanotube/amorphous carbon composite systems were compared to those of otherwise equivalent continuous CNT composites using ReaxFF reactive molecular dynamics simulations. The simulation results quantify the dependence of composite mechanical properties on the number of nanotube-matrix