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Molecular Dynamics Modeling of Carbon Nanotube Composite Fracture using ReaxFF BENJAMIN JENSEN, KRISTOPHER WISE, NASA Langley Research Center, GREGORY ODEGARD, Michigan Technological University — Carbon nanotube (CNT) fiber reinforced composites with specific tensile strengths and moduli approaching those of aerospace grade carbon fiber composites have recently been reported. This achievement was enabled by the emerging availability of high N/tex yarns in kilometer-scale quantities. While the production of this yarn is an impressive advance, its strength is still much lower than that of the individual CNTs comprising the yarn. Closing this gap requires understanding load transfer between CNTs at the nanometer dimensional scale. This work uses reactive molecular dynamics simulations to gain an understanding at the nanometer scale of the key factors that determine CNT nanocomposite mechanical performance, and to place more realistic upper bounds on the target properties.

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