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Adhesion and Reinforcement in Carbon Nanotube Polymer Composite CHENYU WEI, NASA Ames Research Center — The temperature dependent adhesion behavior and reinforcement in carbon nanotube(CNT)-polymer (polyethylene) composite is studied through molecular dynamics (MD) simulations. The interfacial shear stress through van der Waals interactions is found to increase linearly with applied tensile strains along the nanotube axis direction, until the non-covalent bonds between CNTs and molecules break successively. A lower bound value about 46 MPa is found for the shear strength at low temperatures. Direct stress-strain calculations show significant reinforcements in the composite in a wide temperature range, with $\sim$ 200% increase in the Young's modulus when adding 6.5% volume ratio of short CNTs, and comparisons with the Halpin-Tsai formula are discussed.

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