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Structural ordering in nanotube polymer composites CHENYU WEI, DEEPAK SRIVASTAVA, NASA Ames Research Center, K.J. CHO, Mechanical Engineering Department, Stanford University — The structural and mechanical properties of polymeric carbon nanotube (CNT) composites have been studied through molecular dynamics simulations. Polymer molecules (polyethylene in this study) have been found to form layer structures around the nanotube with oscillating features and with orientations aligned with the tube axis. The increase of the structural order parameter of orientations $<S_Z>$ is shown to contribute to the enhancement of mechanical modulus of CNT based composites. $<S_Z>$ is found to increase with applied strains, and the corresponding structural change of the composite is shown to be inelastic, which is not fully recovered upon removal of the applied strains.

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