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Mechanical properties and deformation mechanisms of collapsed carbon nanotubes fibers by coarse-grain molecular dynamic simulations

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Continuous carbon nanotube (CNT) fiber is made of CNT bundles where most CNTs are well-aligned along the fiber axis direction and wavy CNT threads filled between bundles. Meso-scale model of carbon nanotube (CNT) fiber was built through shape-based coarse-graining approach. Simulations of monotonic and cyclic loading/unloading tests were conducted to study mechanical properties and meso-structural evolution of the CNT fiber. Contributions of CNT bundles and wavy threads on mechanical properties of CNT fibers under tensile loading were investigated as well. The key factors that determine the mechanical properties of the CNT fibers were investigated: inter-bundle interaction dominates at low strain-rates, and mechanical characteristic of CNT bundles dominates at high strain-rates.

Keywords: Carbon nanotube fibers, Collapsed carbon nanotubes, Shape-based coarse-graining, Meso-scale molecular dynamics, Hierarchical structure