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Mesoscopic simulations of mechanical and thermal transport properties of carbon nanotube films[1]

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The behavior of carbon nanotube (CNT) materials subjected to mechanical loading exhibits a number of fascinating effects caused by collective interactions among individual CNTs. This work is aimed at revealing the microstructural mechanisms of deformation of CNT films and variation of their thermal transport properties in simulations based on a recently developed mesoscopic model. The mesoscopic model accounts for stretching, bending and buckling of individual nanotubes, van-der Waals interaction and existences of cross-links between CNTs, their intrinsic thermal conductivity, contact heat transfer between nanotubes, and finite conductance of bending buckling kinks. Mechanical properties of CNT films with continuous networks of bundles subjected to compressive and tensile loading are studied in dynamic simulations. The deformation-induced variations of structure are analyzed depending on the CNT length, material density, density of cross-links, and structural parameters of the CNT networks. The scaling laws of the effective thermal conductivity of CNT films with respect to the nanotube length and material density are established and compared with theoretical predictions.

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