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Multiscale Modeling of Heat Conduction in Carbon Nanotube Aerogels FENG GONG, DIMITRIOS PAPAVASSILIOU, University of Oklahoma, HAI DUONG, National University of Singapore — Carbon nanotube (CNT) aerogels have attracted a lot of interest due to their ultrahigh strength/weight and surface area/weight ratios. They are promising advanced materials used in energy storage systems, hydrogen storage media and weight-conscious devices such as satellites, because of their ultralight and highly porous quality. CNT aerogels can have excellent electrical conductivity and mechanical strength. However, the thermal conductivity of CNT aerogels are as low as 0.01-0.1 W/mK, which is five orders of magnitude lower than that of CNT (2000-5000 W/mK). To investigate the mechanisms for the low thermal conductivity of CNT aerogels, multiscale models are built in this study. Molecular dynamic (MD) simulations are first carried out to investigate the heat transfer between CNT and different gases (e.g. nitrogen and hydrogen), and the thermal conductance at CNT-CNT interface. The interfacial thermal resistances of CNT-gas and CNT-CNT are estimated from the MD simulations. Mesoscopic modeling of CNT aerogels are then built using an off-lattice Monte Carlo (MC) simulations to replicate the realistic CNT aerogels. The interfacial thermal resistances estimated from MD simulations are used as inputs in the MC models to predict the thermal conductivity of CNT aerogels. The volume fractions and the complex morphologies of CNTs are also quantified to study their effects on the thermal conductivity of CNT aerogels. The quantitative findings may help researchers to obtain the CNT aerogels with expected thermal conductivity.

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