

Abstract Submitted  
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**Thermal conductivity of polymer nanocomposites** DI XU, DILIP GERSAPPE, Dept of Materials Science and Engg, Stony Brook University, Stony Brook NY 11794 — Carbon nano-materials have been extensively used to improve the properties of a polymer matrix. Among them, carbon nanotube and graphene have superior thermal conductivity, which could greatly enhance the thermal behavior of polymers. The effects of carbon fillers, however, depend on factors such as filler concentration, and compatibility with polymer matrix. We used molecular dynamic simulations to study how these factors would affect the thermal behavior of carbon-polymer composites, with a focus on carbon nanotube based composites and graphene based composites. We validated our methods by testing thermal conductivity of water, which agreed well with published experiment values. By using our model, we explore how the filler concentration, and how the coupling energy between two phases could affect the thermal performance of polymer matrix. We also test the effects of filler orientation and compare the different performance of carbon nanotube and graphene in improving the thermal conductivity of composites. The results provide guidelines to design carbon-based polymer composites with better thermal properties.

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