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Multiscale prediction of thermal conductivity for nanocomposites containing crumpled carbon nanofillers with interfacial characteristics

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Abstract

The importance of the thermal conductivity of engineering plastics reinforced with nanofillers is increasing in various industries, and the need for a model with which to make reliable predictions continues. We propose a micromechanics-based multiscale model that considers multi-shaped nanofillers to predict the thermal conductivity of composites. The distribution of each phase is assumed to be probabilistically distributed, and the Kapitza resistance at the interface between the filler and matrix was calculated by means of a molecular dynamics simulation. A polybutylene terephthalate (PBT) composite system embedded with multi-walled carbon nanotubes (MWCNTs) was used

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