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Effective Thermal Properties and Thermal Boundary Resistances of Multiphase Composites Containing Carbon Nanotubes and Inorganic Nanoparticles FENG GONG, National University of Singapore, DIMITRIOS PA-PAVASSILIOU, University of Oklahoma, HAI DUONG, National University of Singapore — Monte Carlo simulations were employed to investigate the effective thermal conductivity  $(K_{\text{eff}})$  and thermal boundary resistances  $(R_{\text{bd}})$  of polymer composites containing carbon nanotubes (CNTs) and inorganic nanoparticles. By considering  $R_{\rm bd}$  between any two phases and the synergistic effect of CNTs and nanoparticles, our model more accurately predicted  $K_{\rm eff}$  of 3-phase composites than effective medium theories (EMTs). Complex morphology of CNTs (diameter, length) and the heat transfer at interfaces  $(R_{\rm bd})$  were quantified to study their influences on  $K_{\rm eff}$ . By matching the simulated  $K_{\rm eff}$  with the measured  $K_{\rm eff}$ ,  $R_{\rm bd}$  of polymer-CNT and polymer-nanoparticle could be estimated. The results showed that  $K_{\text{eff}}$  of composites increases when CNT fraction increases and when  $R_{\rm bd}$  of polymer-nanofillers (CNTs and nanoparticles) decreases. CNT bundle was built to investigate its effect on  $K_{\rm eff}$  of composites, which had not been considered in EMTs. It was found that when CNT bundles increase,  $K_{\rm eff}$  decreases in the composites with random and parallel CNTs, whereas,  $K_{\rm eff}$  increases in those with perpendicular CNTs.

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