MAR07-2006-005433

Abstract for an Invited Paper for the MAR07 Meeting of the American Physical Society

Heat flow at solid-liquid interfaces: confrontation between experiment and simulation DAVID CAHILL, University of Illinois

Heat transport in nanostructures and nanostructured materials provides a novel paradigm for direct comparisons between the results of experiment and simulation. Time-resolved, pump-probe optical techniques enable measurements of the evolution of temperature on time scales from ps to ns. Our pump-probe experiments take two basic forms: measurements of heat transport across planar interfaces using time-domain thermoreflectance and measurements of heat flow from a metal or semiconductor nanostructure into its surroundings using transient absorption. The systems that we are studying are directly accessible to simulation by classical molecular dynamics on the same time and length scales that are encountered in the experiments. Working with our collaborators, P. Keblinski and his colleagues at RPI, we have made quantitative comparisons between experiment and simulation for heat transport from carbon nanotubes and fullerene molecules into a surrounding fluid; and heat transport across hydrophilic and hydrophobic interfaces with water. Any such comparison must take into account i) non-idealities in the experiments; ii) uncertainties in the potentials and atomic geometries in the computational model; and iii) the fact that classical simulations may include high frequency vibrational modes that are not thermally excited in the experiments. Despite the fact that transport at solid-liquid interfaces provide a more reliable system for quantitative comparisons between experiment and simulation.