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Thermal Transport in Carbon Nanotubes JEREMY CHRISTMAN, ANDREW MOORE, MAHFUZA KHATUN, Ball State University — Recent advances in nanostructure technology have made it possible to create small devices at the nanoscale. Carbon nanotubes (CNT's) are among the most exciting building blocks of nanotechnology. Their versatility and extremely desirable properties for electronic and other devices have driven intense research and development efforts in recent years. A review of electrical and thermal conduction of the structures will be presented. The theoretical investigation is mainly based on molecular dynamics. Green Kubo relation is used for the study of thermal conductivity. Results include kinetic energy, potential energy, heat flux autocorrelation function, and heat conduction of various CNT structures. Most of the computation and simulation has been conducted on the Beowulf cluster at Ball State University. Various software packages and tools such as Visual Molecular Dynamics (VMD), Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), and NanoHUB, the open online resource at Purdue University have been used for the research. The work has been supported by the Indiana Academy of Science Research Fund, 2010-2011.

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