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Heat Flux and Thermal Conductivity of Carbon Nanotubes (CNTs) SHAUN WOOD, CHRIS NELSON, MAHFUZA KHATUN, Physics and Astronomy, Ball State University — We report an analysis of heat flux data and thermal conductivity of Carbon Nanotubes (CNTs). These one dimensional (1-D) honeycomb structures are extremely versatile and robust with high thermal and electrical conductivities. They can exist in metallic or semiconducting forms depending on their structures. Successful implementation of such structures will have tremendous technological impacts. The theoretical investigation is based on equilibrium molecular dynamics (EMD) technique where the autocorrelation heat flux functions and the thermal conductivity have been calculated using the Green-Kubo formalism from linear response theory. Two open source codes are used in this investigation. The CNTs are generated using the Visual Molecular Dynamics (VMD) software and the simulations are performed using the code called Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). The code is run on the Beowulf Computing Cluster. Thermal conductivity of CNTs with different lengths and temperatures has been calculated and studied. In addition, the time-dependence characteristics of the heat flux functions have been analyzed, and will be discussed.

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