ABSTRACT

RESEARCH PAPER: Thermal Transport Properties of Carbon Nanotubes

STUDENT: Shaun Wood

DEGREE: Master of Arts

COLLEGE: Sciences and Humanities

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On account of the trend of the latest microelectronic technology to become progressively smaller, it becomes increasingly important to predict the thermal behavior of constituent materials. Among the most promising candidates for use in microelectronics and thermal conductors are carbon nanotubes (CNTs). Thermal properties of such small scale components are difficult to measure experimentally. For this reason, we report the results of our investigation on the thermal conductivities of CNTs. This study is based on an equilibrium molecular dynamics (EMD) approach. The thermal conductivity has been calculated using the Green-Kubo formalism from linear response theory. The molecular dynamics simulations were run on a Beowulf Computing Cluster using open source software called Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). Thermal conductivity for CNTs of various lengths has been calculated and studied. In addition, the time-dependence characteristics of the heat flux functions have been analyzed, and will be discussed.