ABSTRACT

THESIS: The thermal properties of Single-Walled Carbonanotubes

STUDENT: Tuan A. Le

DEGREE: Master of Science

COLLEGE: Sciences and Humanities

DATE: May 2019

PAGES: 60

Carbon Nanotubes (CNTs) are extremely versatile and robust with their high electrical and thermal conductivity and mechanical strengths. They might be metallic and/or semiconducting depending on their chirality. This study focuses mainly on thermal properties of Single Walled Carbon Nanotubes (SWCNTs), which can be characterized by the shape of their edges, armchair, zigzag or chiral type.

Thermal conductivity and heat flux autocorrelation function are obtained using Green-Kubo formalism. The formalism is a statistical and computational solution of phonon transport equation. The Nose Hoover thermostat and the Tersoff potential are incorporated in the simulator.

Three open source codes have been used in this investigation. These include: Visual Molecular Dynamics (VMD), Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), and Dynamical matrix code. The numerical computation for the thermal conductivity is based on equilibrium molecular dynamics (EMD) technique. Ball State Beowulf Cluster and Wolfram Mathematica serves as a platform on which all results are obtained.