Abstract Submitted for the OSF11 Meeting of The American Physical Society

Thermal Transport in Carbon Nanotubes using Molecular Dynamics ANDREW MOORE, MAHFUZA KHATUN, Ball State University — We will present results of thermal transport phenomena in Carbon Nanotube (CNT) structures. CNTs have many interesting physical properties, and have the potential for device applications. Specifically, CNTs are robust materials with high thermal conductance and excellent electrical conduction properties. A review of electrical and thermal conduction of the structures will be discussed. The research requires analytical analysis as well as simulation. The major thrust of this study is the usage of the molecular dynamics (MD) simulator, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). A significant investigation using the LAMMPS code is conducted on the existing Beowulf Computing Cluster at BSU. NanoHUB, an open online resource to the entire nanotechnology community developed by the researchers of Purdue University, is used for further supplementary resources. Results will include the time-dependence of temperature, kinetic energy, potential energy, heat flux correlation, and heat conduction.

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