Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

First principles calculations of thermal phonon transport in nanostructures THUSHARI JAYASEKERA, North Carolina State University, A. CALZOLARI, CNR-INFM DEMOCRITOS National Simulation Center c/o Sincrotrone Trieste - SS14, Km 163,5 Basovizza, I-34012 TRIESTE, Y.F. CHEN, K.W. KIM, M. BUONGIORNO NARDELLI, North Carolina State University — As the size of the electronic devices gets smaller, the power density associated with the devices becomes a very significant aspect that requires a great attention. The devices need to be designed in such a way that the heat removal from the system is efficient, thus, it is very important to understand the heat transport at the nanoscale for better thermal management. In this talk, we will discuss recent advances in the development of efficient techniques to compute the phonon contributions to thermal conductance from first principles. We will show examples of prototypical applications, ranging from atomic chains to graphene nanoribbon junctions and constrictions This work was supported, in part, by the NERC/NIST SWAN-NRI and the DARPA/HRL CERA programs.

Thushari Jayasekera
North Carolina State University

Date submitted: 28 Nov 2009 Electronic form version 1.4