Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Thermal conductivity and rectification study of restructured Graphene ANUJ ARORA, University of Tokyo — Electronics' miniaturization, has led to search for better thermal management techniques and discovery of important transport phenomenon. Thermal rectification, directionally preferential heat transport analogous to electrical diode, is one such technique, garnering tremendous interest. Its possibility has been explored through structural asymmetry, introducing a differential phonon density of states in hot and cold regions. As of now, mass and shape asymmetries have been studied, both experimentally and theoretically. However, strict requirements of material length being shorter than phonon mean free path and phonon coherence preservation at surface, makes connecting two materials with different temperature-dependent thermal conductivities, a more natural approach. To avoid resultant thermal boundary resistance and integration complexities, we achieve the affect in single material, by restructuring a region of Graphene by introducing defects. The asymmetry impedes ballistic phonon transport, modulating temperature dependence of thermal conductivity in the two regions. We perform deviational Monte Carlo simulations based on Energy-based formulation to microscopically investigate phonon transport, possibility and optimal conditions for thermal rectification. The proposed method uses phonon properties obtained from first principle, treat phonon-boundary scattering explicitly with properties drawn from Bose-Einstein Distribution.

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Date submitted: 05 Nov 2015 Electronic form version 1.4