

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Nanoscale Thermal Transport in Graphene Interfaces

RUI MAO, BYOUNGDON KONG, North Carolina State University, THUSHARI JAYASEKERA, Southern Illinois University, MARCO BUONGIORNO-NARDELLI, KI WOOK KIM, North Carolina State University, NORTH CAROLINA STATE UNIVERSITY TEAM — We have investigated nanoscale thermal transport in epitaxial graphene systems using first-principles calculations and the Landauer formalism for phonon transport. Two types of interfaces are investigated: graphene-dielectric and graphene-metal heterojunctions. Hexagonal boron nitride (h-BN), SiC and SiC with hydrogen passivation (SiC-H) are studied as potential dielectric substrate materials for graphene devices. As for graphene-metal contacts, we have considered Au and Ti as prototypical systems for physisorbed and chemisorbed metal contacts, respectively. The interfacial thermal resistances of h-BN/G system is $5.3 \cdot 10^{-9}$ Km^2/W at room temperature, which is approximately one order of magnitude smaller than that of SiC/G system ($55\text{-}79 \cdot 10^{-9}$ Km^2/W). Further analysis shows that heat conduction at the graphene interfaces is dominated by low-lying acoustic phonons and the thermal resistances strongly depend on atomic details at the interface such as lattice mismatch, disorder and surface reconstruction. Our work demonstrates the importance of developing a microscopic description of phonon dynamics at heterogeneous interfaces to engineer and design devices with optimal thermal management.

Rui Mao
North Carolina State University

Date submitted: 28 Nov 2011

Electronic form version 1.4