Efficient Nanoscale Thermal Transport for Electronics Cooling

OBJECTIVES

Linear and Nonlinear Thermal Transport in Graphene and Graphene Nanoribbons (GNRs)

- Decomposition of κ of supported or suspended graphene into different phonon modes.
- Thermal rectification in GNRs.

Thermal Transport across CNT /GNR – nonmetal and CNT /GNR – metal Interfaces

- Atomic scale simulations on thermal transport across CNT/GNR – nonmetal/metal interface.

METHODS

Density Functional Theory

- Explore the nature of bonding at CNT/GNR – Si interface.

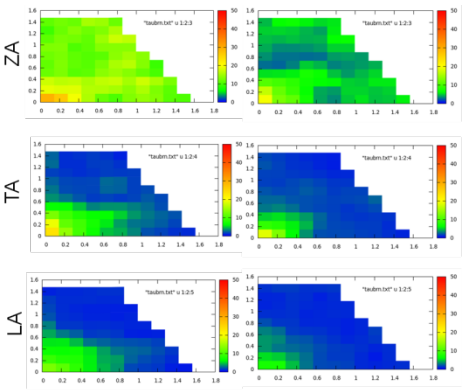
Classical MD Simulations

- Capture the nature of phononic heat transport in nonmetals.

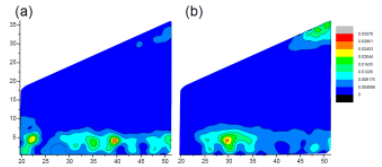
Two-temperature MD Simulations

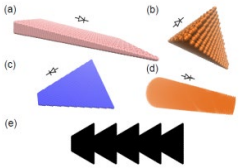
- Capture electron-phonon coupling as well as phonon-phonon coupling in a single simulation on nonmetal – metal interface thermal transport.

KEY RESULTS AND FINDINGS:

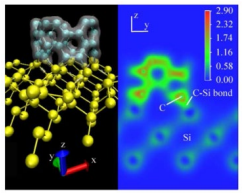


Contribution to thermal transport in suspended/supported graphene from different phonon branches.

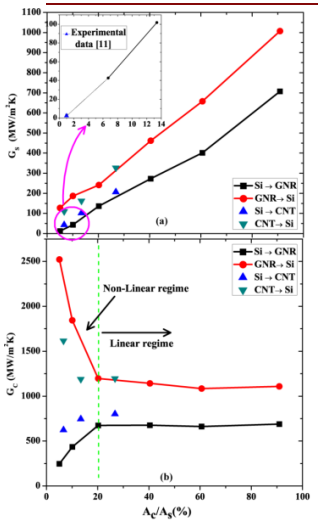


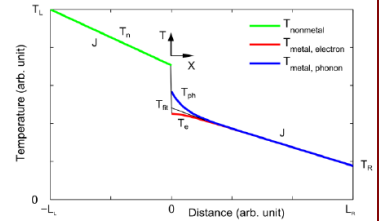


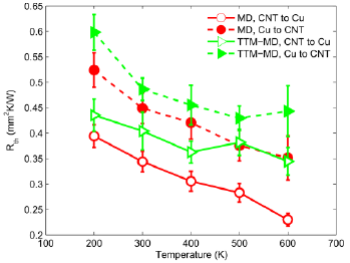
Phonon localization at the edge/surface of nanostructures leads to asymmetric thermal transport, i.e., thermal rectification.



With a better understanding of the nature of bonding at GNR/CNT – Si interface from DFT, better agreement with experiment was achieved.







Two-temperature MD predicts higher interfacial thermal resistance than conventional MD, which agrees with experimental values better.

QUANTITATIVE IMPACT

Impact

- First to conduct spectral decomposition of κ of suspended and supported graphenes, and successfully revealed the strong effect of graphene-substrate coupling.
- First two-temperature MD simulations on interfacial thermal transport including both electron and phonon degree of freedom.

Applications

- Better understanding of 2D thermal transport in suspended/supported graphenes.
- Development of thermal rectifiers with high κ.
- Development of excellent thermal interface materials (TIM) using CNT and GNR.

Selected Publications:

- Wei, Bao, and Ruan, *Nano Energy* 71, 104619 (2020).
- Sullivan, Vallabhaneni, Kholmanov, Ruan, Murthy, and Shi, *Nano Lett.* 17, 2049−2056 (2017)