Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Thermal Conductivity of Twisted Bilayer Graphene Nanoribbons from Non-equilibrium Molecular Dynamics Study.[1] CHENYANG LI, SHANSHAN SU, SUPENG GE, ROGER LAKE, University of California - Riverside — Misorientation of the two layers of bilayer graphene affects both the electronic properties and the vibrational modes or phonons. The phonon density of modes is little affected by misorientation, however, zone-folding can allow new Umklapp scattering processes that could affect the phonon transport and thermal conductivity. To investigate this, we use NEMD molecular dynamics simulations as implemented in LAMMPS to study the thermal conductivity of the misoriented graphene bilayers. Seven commensurate misorientation angles varying from 6.01 to 48.36 have modeled and analyzed to understand how the misorientation angle affects the thermal conductivity of relatively wide (˜10 nm) misoriented bilayer graphene nanoribbons (m-BLGNRs). Within numerical accuracy, we find that the thermal conductivity of the m-BLGNRs for all of the simulated commensurate angles have the same thermal conductivity with AB stacked and AA stacked BLGNRs. These results indicate that neither the misorientation angle nor the stacking order affect the thermal conductivity of BLGNRs.

[1]This work was supported as part by the NSF 1307671.

Chenyang Li
Univ of California - Riverside

Date submitted: 10 Nov 2016 Electronic form version 1.4