Engineering Thermal Conductivity in Graphene Nanostructures: a Molecular Dynamics Study

Jiuning Hu
School of Electrical and Computer Engineering, West Lafayette, IN, U.S.A.

Xiulin Ruan
School of Mechanical Engineering, West Lafayette, IN, U.S.A.

Yong P. Chen [C, S]
Department of Physics, Birck Nanotechnology Center and School of Electrical and Computer Engineering, West Lafayette, IN, U.S.A.

We have used molecular dynamics to calculate the thermal conductivity of various graphene based nanostructures. For symmetrical graphene nanoribbons, the calculated thermal conductivity is on the similar order of magnitude of the experimentally measured value for graphene. We have investigated the effects of edge chirality and found that nanoribbons with zigzag edges have considerablly larger thermal conductivity than that of nanoribbons with armchair edges. For asymmetric nanoribbons, we have found considerable thermal rectification. For example, for a 6nm-long triangular shaped nanoribbon, the thermal conductivity from the wider end to the narrower end is over 2 times that from the narrower to the wider end. We also studied the effects of defects and found that vacancies in the ribbons can significantly decrease the thermal conductivity and the thermal rectification is robust with edge roughness. We have also studuied the vertical thermal transport and interface thermal resistance of graphene on various substrates. Our results can be valuable for heat management in graphene nanoelectronics and nanoscale thermal engineering.