140f Ballistic Heat Transport in One-Dimensional and Quasi-One-Dimensional Nanostructures

Chia-Yi Chen and Dmitry I. Kopelevich

The steady decrease of the feature size of integrated circuits towards the nanometer scale leads to an increase in generated heat per unit area. Hence, efficient transfer of heat away from hotspots of integrated circuits becomes a crucial issue in the performance, stability, and design of new generations of electronic devices. The importance of efficient thermal transport is even more pronounced in moving parts of nanoelectromechanical systems (NEMS). Recent research has shown that low-dimensional nanomaterials possess high thermal conductivity and hence are promising candidates for efficient heat reduction in nanodevices.

In this talk, we present results of theoretical modeling and molecular dynamics (MD) simulations of heat transport in one-dimensional (long chain molecules) and quasi-one-dimensional (carbon nanotubes) nanostructures. The study is performed under the assumption that the contribution of electrons to thermal conductivity is negligible and therefore the heat transfer is solely due to nonlinear interactions between vibrations of atoms in a nanostructure. One of the challenges of modeling nanoscale heat transport is the failure of the continuum thermal conductivity equation at this small scale. In part, the continuum models fail because the mean free path of heat carrying phonons (wave packets of linear lattice vibrations) exceeds the characteristic sample size. Hence, the dominant mechanism of the heat transport in nanoscale systems is the ballistic motion of heat carriers in contrast with the diffusive heat transport in bulk materials. Moreover, there is increasing evidence (both theoretical and experimental) that, in addition to phonons, intrinsic nonlinear lattice vibration modes play an important role in heat transport in low-dimensional nanoscale systems.

We investigate the role of various nonlinear lattice vibration modes in the heat transport process. In the initial stage of our analysis we obtain the steady-state nonlinear lattice vibration modes and investigate stability and mobility of these individual modes. The steady-state modes are obtained using the rotating wave approximation and their stability is analyzed using the Floquet theory. We observe highly localized nonlinear vibration modes (known as breathers) which have properties qualitatively different from the linear phonons.

We further investigate the role of the breathers by performing MD simulations in a system with a thermal gradient imposed by coupling two ends of the one-dimensional nanostructures to thermal baths at different temperatures. The MD simulations reveal the evolution of the vibration modes and show that the stable breathers exist for a very long time and, at certain conditions, they move at a high constant velocity. This property of breathers suggests their potential for efficient transfer of heat away from hotspots in a nanoscopic device.