Thermal transport in graphene nanorings using molecular dynamics simulations

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Understanding heat transport in nanoscale systems has become a crucial issue in recent years. The increased levels of dissipated power in ever smaller integrated circuits make the search for high thermal conductors essential. Thermoelectric energy conversion, in contradistinction, requires materials with a strongly suppressed thermal conductivity, but still high electronic conduction. Graphene occupies a unique place amongst materials in terms of its thermal properties. It posseses one of the highest thermal conductivities but that can be greatly reduced in graphene nanoribbons (GNR) [1]. Since graphene is a promising candidate for superseding silicon in future nanoelectronics, understanding how heat is carried in different GNR structures is important. Among these structures, graphene rings stand out because of the straightforward way in which they exploit quantum intereference effects. These effects could be used for the design of new quantum interferometers or spintronic devices. We recently demonstrated that graphene rings might be useful as thermoelectric devices too due to their high Seebeck coefficient and thermoelectric figure of merit when heat is only carried by electrons [2]. Yet, lattice heat conduction, which is the most important contribution to heat transport in graphene due to the strong covalent sp^2 bonding, has not been studied.

In this work, we use non-equilibrium molecular dynamics (NEMD) simulations as implemented in the LAMMPS package to study lattice heat conduction in graphene rings. NEMD simulations provide a direct method to calculate lattice thermal conductivity by introducing a heat flow, obtaining a temperature gradient accross the system, and then, using Fourier's law [3]. We compare thermal conductivities for perfect graphene ribbons and rectangular graphene rings of widths up to 5 nm in a wide range of temperature. Our results show that thermal conductivity in rings is greatly reduced as compared to the corresponding ribbon for all considered widths, being the reduction stronger for narrow ribbons and low temperatures.

References

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Figures

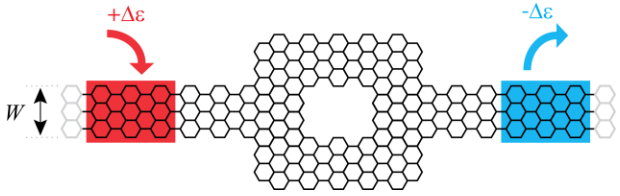

Figure 1: Schematics of a graphene nanoring. Red (blue) area represents the hot (cold) contact, where an amount of energy $\Delta\varepsilon$ is introduced (removed) every timestep.