Strong reduction of the lattice thermal conductivity in graphene rings

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Graphene occupies a unique position because of its extremely high electric σ and thermal κ conductivities. However, thermoelectric applications demand high σ but low κ. Nanotechnology paves the way to achieve this goal. Lattice thermal conductivity of graphene systems can be greatly reduced by rough edges, H-passivation and patterning. Among graphene structures, nanorings stand out because of the straightforward way in which they exploit electronic quantum interference effects, which could be used for designing new thermoelectric devices, as we demonstrated when heat is only carried by electrons [1].

In this work, we address the contribution of the atomic lattice to heat transport in graphene nanoribbons and nanorings by using two different approaches. For temperatures above 100 K (roughly 1/3 of the Debye temperature), we use non-equilibrium molecular dynamics, while for lower temperatures we apply a combination of density functional-based tight-binding and Green's functions. We consider nanoribbon widths up to 6 nm, several ring configurations as well as the effects of rough edges. Our results show that graphene nanorings can efficiently suppress the lattice thermal conductivity as compared to nanoribbons, especially at low temperatures. Furthermore, we demonstrate rough edges have only a weaker impact on the heat transport in nanorings [2].

References

[1] M. Saiz-Bretín, A. V. Malyshev, P. A. Orellana and F. Domínguez-Adame, Phys. Rev. B **91**, 085431 (2015).
[2] M. Saiz-Bretín, A. V. Malyshev, F. Domínguez-Adame, D. Quigley and R. A. Römer, Carbon **127**, 64 (2018).

Figures

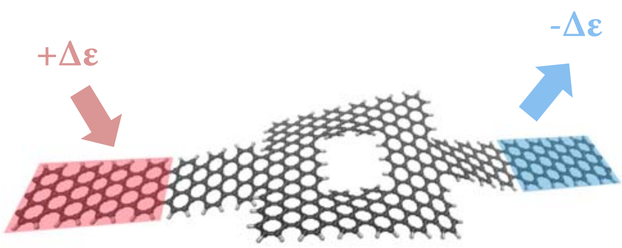

Figure 1: Schematics of a graphene ring. Red/blue areas represent hot/cold contacts, where an amount of energy $\Delta\varepsilon$ is added/subtracted each time step.

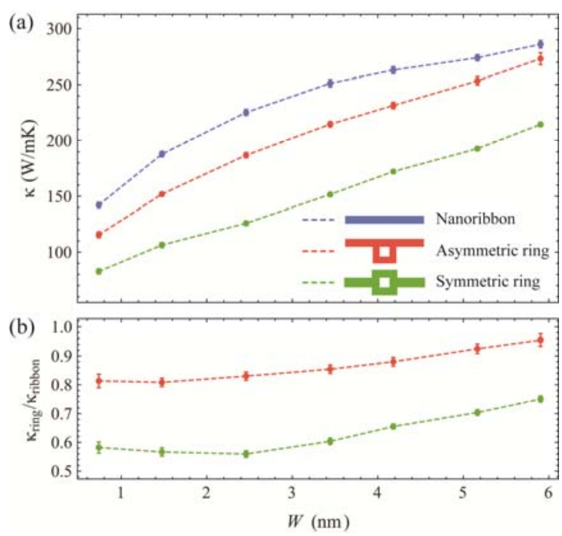

Figure 2: Thermal conductivity as a function of the ribbon width, *W*.