Lattice Thermal Transport in Nanocrystalline Graphene

K.R. Hahn[1], C. Melis[1] and L. Colombo[1]*

[1] Department of Physics, University of Cagliari – Cittadella Universitaria, 09042 Monserrato (Ca), Italy
[*]luciano.colombo@unica.it

Approach-to-equilibrium molecular dynamics (AEMD) simulations [1] have been used to study lattice thermal transport in nanocrystalline graphene.
At first, a computational protocol is reviewed, which is able to generate nanostructured graphene samples with unprecedented size and different topology [2]. Then, we investigate their structure and phonon spectrum, as well as the corresponding average mean free path of heat carriers. Finally, thermal conductivity is predicted as a function of grain size, number of defect atoms at grain boundaries, bond network and grain topology [3]. A comparison with pristine graphene [4] is worked out in order to enlight the role of grain boundaries.
A resulting picture is elaborated, that thermal transport in nanostructured graphene can be described by an effective connection in series of conducting elements and resistances. Phonon scattering effects (at grain boundaries) are included into a boundary resistance term, while the conductivity of crystalline domains is approximated by the thermal conductivity of a defect free lattice with same grain size.

References

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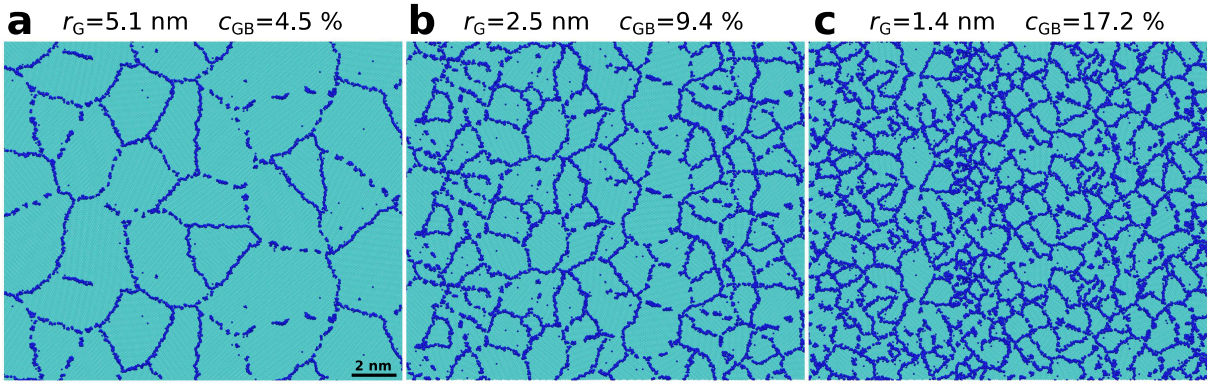

Figure 1: Simulation cells of nanocrystalline graphene with a mean radius of gyration of (a) 5.1, (b) 2.5 and (c) 1.4 nm. Atoms assigned to the grain boundary are indicated in blue.

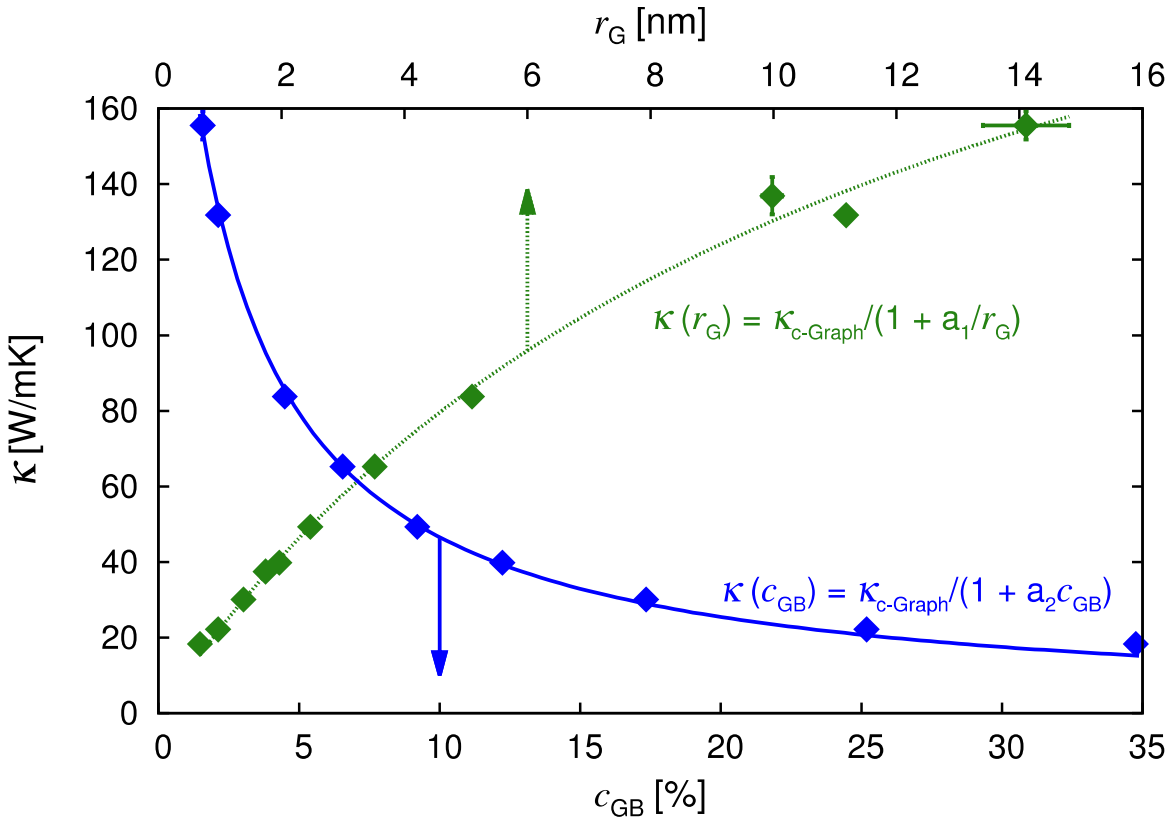

Figure 2: Thermal conductivity of nanocrystalline graphene κ as a function of the concentration of atoms in the grain boundary $\kappa(c_{GB})$ (blue solid line) and of the gyration radius $\kappa(r_G)$ (green dotted line) of grains.