Real-size impact on the thermal conductivity of nanostructures by approach-to-equilibrium molecular dynamics

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The reduction of thermal conductivity measured in nanostructures, films or wires, is also observed in atomistic simulations using the molecular dynamics method. However, the sizes affordable to approaches that exploit the stationnary regime, such as the Green-Kubo or the direct methods, are drastically smaller than the dimensions of the nanowires fabricated by top-down or bottom-up approach. Moreover in the case of membranes, the period of the nanostructuration by holes can be only small in front of the possible achievements by nanofabrication. In former studies[1] [2] we have used a heat transient method, called approach-to-equilibrium molecular dynamics (AEMD). The AEMD permits to study larger systems periodised in the 3 directions to mimic bulk materials of thermal conductivity ranging from 1 to several hundreds of W/(K.m). In the present work, we demonstrate that AEMD can also be applied to calculate the thermal conductivity of 1D or 2D systems having very large dimensions. In the case of nanowires, we show that very long phonon mean free paths still persist in wires of diameter up to 15 nm whenever their surface is smooth. We also study membranes in presence or not of a nanostructuration formed of holes, with the same diameter and step that is used to fabricate membranes dedicated to thermolectric devices (see Fig1). The reduction of thermal conductivity obtained from the nanostructuration is in agreement with latest experiments.

FIG. 1: Atomistic simulation box of a nanostructured membrane. The distance between the hole centers is equal to 60 nm, the radius of the holes is $\approx$ 11 nm.

[1] E. Lampin, P. L. Palla, P.-A. Francioso and F. Cleri, J. Appl. Phys. **114**, 033525 (2013)

[2] H. Zaoui, P. L. Palla, F. Cleri and E. Lampin, *Length dependence of thermal conductivity by approach-to-equilibrium molecular dynamics*,submitted to Phys. Rev. B