Nanoscale Heat Transfer via Ab-Initio Monte Carlo Simulation

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It is challenging to accurately model the heat transfer in devices of characteristic length close to the phonon mean free path, i.e. when the Fourier's heat transport formalism reaches its limits [1]. Additionally, if the lateral size of the structure also reaches the nanoscale, the role of the phonon reflections at the external interfaces becomes of high importance. A stochastic resolution of the Boltzmann's transport equation for phonons (pBTE) based on particle Monte Carlo (MC) algorithm is very efficient in terms of computational resources in the case of complex systems [2].

In this work, an original versatile particle MC simulator in which the material parameters, i.e. phonon dispersion and scattering rates, are parametrized by using ab initio calculation [3] is presented. It is a Full-band simulator since both dispersion and scattering rates are computed in the entire 3D Brillouin zone. To model the effect of rough external interfaces on the phonon transport, a combination of specular and diffuse phonon reflections at the external rough interfaces has been implemented in the phase space [4].

Rough nanowires and thin films schematized in Fig.1 were investigated. Cubic (Si3C) and hexagonal (Si2H) Silicon have been implemented in our MC code by using a Full-band approach, as illustrated for instance by equi-energy maps plotted in Fig 2. The effective thermal conductivity is plotted as a function of length and width in Fig. 3, illustrating the transition from a ballistic regime in short devices to a diffusive regime in long devices and the influence of the rough interfaces. In Fig. 4, the thermal conductivity of films of different phases and orientations of Si are investigated in terms of thermal conductivity and angular distribution of the density of states (DOS). It shows that the main direction of the thermal flux in Si3C is [100] though the flux along the directions [111] and [110] are also significant.

Finally, this coupling between MC and *ab-initio* methods overcomes the main limitation of the MC approach since it allows us to study of a large set of phases and materials along any transport direction without the use of any empirical parameter.

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[3] L. Chaput, et al., Appl. Phys. Lett. **112**, 033104 (2018)
[4] B. Davier, et al, J. Phys.: Condens. Matter, **30**, 4959 (2018)

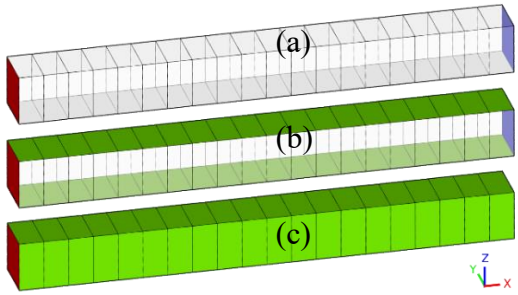

Fig.1: (a) CP nanofilm in cross-plane configuration, (b) IP nanofilm in in-plane configuration, (c) rough nanowire. Transparent/green faces for specular/rough boundaries.

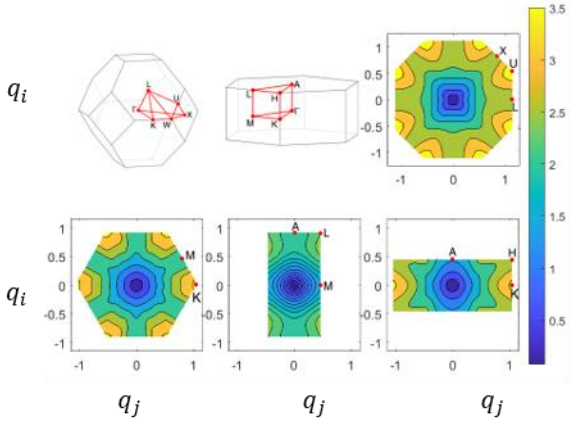

Fig.2: Schema of the BZ in (a) Si3C, (b) Si2H. Equi-energy maps in (c)the (110) plane of Si3C, (d),(e),(f) in planes of Si2H.

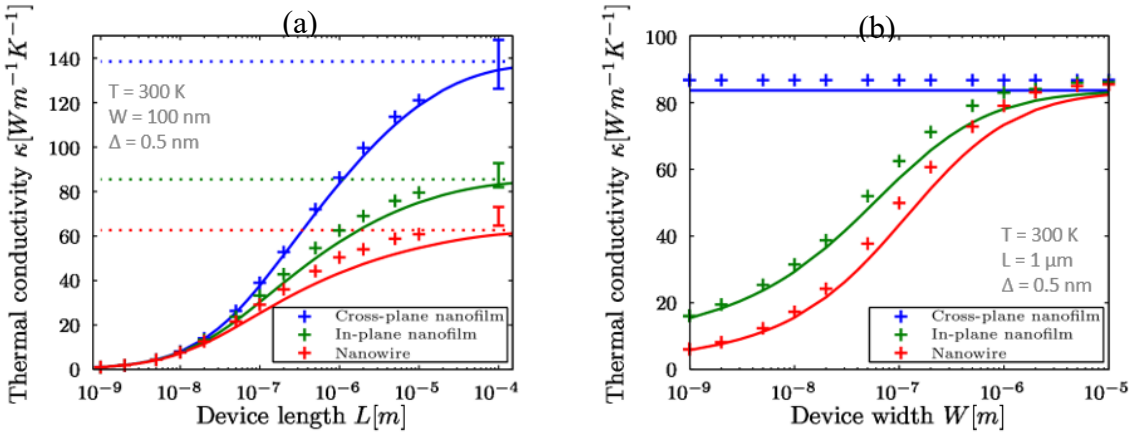

Fig.3: Thermal conductivity κ as a function of (a) length L and (b) width W for IP and CP nanofilms and for nanowires of [100] Si3C.. Dotted lines: long-device conductivity.

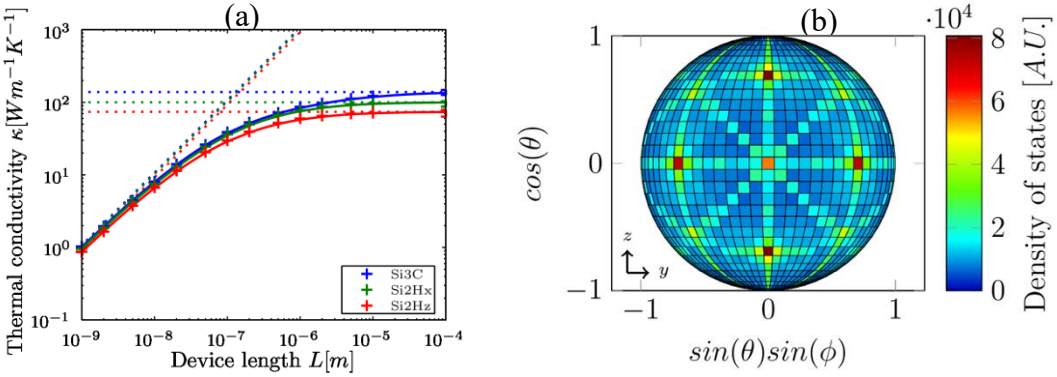

Fig.4: (a) Thermal conductivity as a function of length L for cross-plane nanofilms of Si3C, Si2Hx and Si2Hz. (b) Angular distribution of the DOS in Si3C. θ and ϕ: Polar and azimuthal angles.