Andrea Cepellotti

andrea.cepellotti@epfl.ch

EPFL STI IMX THEOS
MXC 319 (Bâtiment MXC)
Station 12
CH-1015 Lausanne
Switzerland

Thermal Conductivity of Graphene and Graphite: Collective Excitations and Mean Free Paths

We compute the thermal conductivity of single- and bi-layer graphene and graphite by solving exactly the linearised Boltzmann Transport Equation (BTE) for phonons [1], with the phonon-phonon collision rates obtained from density-functional perturbation theory. As previous works found for graphene, we find that the single-mode relaxation time approximation (SMA) cannot describe the in-plane heat transport correctly also in graphite, severely underestimating the thermal conductivity and heat mean free paths. Instead, we show that the exact self-consistent solution of the BTE provides results in good agreement with the experimental measurements [2,3]. The shortcomings of the SMA lie in the assumption that heat flow is transferred only by individual phonon excitations, whereas in layered materials the transport can only be explained in terms of collective phonon excitations. The characteristic length of these collective excitations in graphene is much larger than the experimental samples - as a result, even Fourier's law become questionable, since its statistical nature makes it applicable only to systems larger than a few mean free paths. Moreover, the mean free paths are long but finite, so that the thermal conductivity does not diverge for infinitely large systems. Finally, we analyze in details the effect of isotopes and strain in graphene, often deemed to be responsible for discrepancies between experiments.

References:

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