Emergent Behavior in Thermal Transport

Andrea Cepellotti

University of California, Berkeley, and Lawrence Berkeley National Laboratory, USA

Theory and simulation of materials (THEOS) and National Center for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Switzerland

The thermal conductivity of insulating crystals originates from the energy transfer through lattice vibrations, as commonly described by the phonon Boltzmann transport equation. Since the pioneering work of Peierls, the prevalent hypothesis is that phonons are the heat carriers. However, it has long been known that this picture has shortcomings. For example, in materials of reduced dimensionality [1] or at cryogenic temperatures, the scattering dynamics is dominated by momentum conserving – normal – processes, as opposed to momentum dissipating – Umklapp – processes. In these circumstances, heat flux is not lost at every scattering event. Instead, scattering shuttles heat flux through multiple phonon states, coupling them. As a result, the behavior of the interacting phonon system can be strikingly different from that of its constituents and collective phonon excitations arise [2] causing exotic phenomena: in 2D materials, they are responsible of high thermal conductivities and hydrodynamic behaviors, such as second sound [1,3], where temperature propagates as a damped wave, a phenomenon hitherto observed only in a few materials at cryogenic temperatures. Recently, we rationalized these properties by introducing a gas of collective phonon excitations, called 'relaxons' [4]. Defined as the eigenvectors of the scattering matrix, relaxons allow for a simple - yet exact - interpretation of thermal conductivity in terms of a kinetic gas theory, where the relevant gas is made of such relaxons, the true heat carriers, and not phonons. These considerations provide a new explanation of the high conductivities of 2D materials, revise the time evolution of thermalization processes [5], correct the relevant time and length scale of heat flux dissipation, modify the description of surface scattering, and provide a new viewpoint on semiclassical transport theories.

[1] A. Cepellotti, et al., Nat. Commun. 6, 6400 (2015)
[2] G. Fugallo, et al., Nano Lett. 14, 6109 (2014)
[3] S. Lee et al., Nat. Commun., 6, 6290 (2015)
[4] A. Cepellotti, and N. Marzari Phys. Rev. X 6, 041013 (2016)
[5] J. Hu, et al., PNAS 113, 43, E6555 (2016)