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Wednesday 14th of May 2025 – 14h00

Meeting room – Chemistry Department, ICPM, 1 Bd Arago, Technopôle, Metz

Thermal conductivity, lattice dynamics and phonon lifetime in structurally complex materials

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Understanding the lattice thermal conductivity of materials is of key importance in various fields of material science: for thermoelectric, thermal barriers, thermal transport…. Whereas it is well understood for simple atomic structures, it remains a challenging question for structurally complex materials.

In this presentation I will focus on those materials displaying a 'glass like thermal conductivity' [1], with a relatively small value of the lattice thermal conductivity at ambient temperature and an almost independent temperature dependence in the range 20 to 300 K. This is the case for many different systems such as amorphous materials, disordered periodic crystals [1], clathrates [2], but also aperiodic crystals [3] such as the icosahedral quasicrystal i-AlPdMn [4], and the Rb_2ZnCl_4 phase that displays an incommensurately modulated phase between 190 and 300 K [5].

All these structures can be characterized by what can be named 'structural complexity'. I will first introduce the notion of structural complexity which can be characterized by two main parameters: (i) the long range order and the number of atoms in the unit cell (which goes to infinity for aperiodic crystals); (ii) the disorder that breaks the long range order and may occur as chemical site disorder or lattice displacement, with in the extreme case of amorphous systems the absence of long range order.

I will then review some of the recent results obtained in different materials by combining state of the art inelastic x-ray and neutron scattering with atomic scale simulation. We will show that phonons do not behave at all as in a glass: there is a restricted energy range for which acoustic phonons do propagate, with a rather large mean free path. A simple phonon lattice gaz model as proposed for clathrates [2] can be generalized to interpret the data and resolve the apparent paradoxal findings. The importance of including properly the disorder in large atomic scale simulation will also be discussed [6].

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[3] T. Janssen, G. Chapuis, and M. de Boissieu, *Aperiodic Crystals. From modulated phases to quasicrystals (second edition)* (Oxford University Press, Oxford, 2018), Vol. 20, IUCr Monographs on Crystallography.
[4] M. A. Chernikov, A. Bianchi, and H. R. Ott, Phys. Rev. B **51**, 153 (1995).
[5] D.-M. Zhu and A. C. Anderson, J. Low Temp. Phys. **94**, 117 (1994).
[6] P. F. Lory *et al.*, Phys. Rev. B **102**, 024303, 024303 (2020).

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