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Thermal conductivity and lattice dynamics in structurally complex materials

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The lattice thermal conductivity of many different materials is displaying a 'glass like behavior' [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 disordered crystals [1], for clathrates [2], but also for aperiodic crystals [3] such as the icosahedral quasicrystal i-AlPdMn [4], and the Rb2ZnCl4 phase that displays an incommensurately modulated phase between 190 and 300 K [5]. The detailed understanding of this behavior and the relationship between the phonon spectrum/phonon lifetime and the thermal conductivity is still a matter of debate.
In this presentation I will review some recent results and show how atomic scale simulations of phonon dispersion and phonon lifetime can reproduced the observed experimental data. The structural complexity might be characterized by two main parameters: the long-range order and number of atoms in the unit cell (up to infinity for aperiodic crystals) [6] and the disorder and short rang order. The influence of these two parameters will be discussed [7].

[1] D. G. Cahill, S. K. Watson, and R. O. Pohl, Physical Review B 46, 6131 (1992).
[2] P.-F. Lory et al., Nature Communications 8, 491 (2017).
[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, Physical Review B 51, 153 (1995).
[5] D.-M. Zhu and A. C. Anderson, J. Low Temp. Phys. 94, 117 (1994).
[6] M. de Boissieu et al., Nature Materials 6, 977 (2007).
[7] P. F. Lory et al., Physical Review B 102, 024303, 024303 (2020).

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