

Thermal conductivity and lattice dynamics in structurally complex materials

Thursday, September 15, 2022 9:00 AM (45 minutes)

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 reproduce 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 range order. The influence of these two parameters will be discussed [7].

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