Phonon and phason modes in hypermaterials

Marc de Boissieu

Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, F-38000 Grenoble France

e-mail: marc.de-boissieu@simap.grenoble-inp.fr

The lattice dynamics of simple periodic crystals is described by Bloch waves and phonon quasi-particles, within the first Brillouin zone. There are 3N different modes, where N is the number of atoms in the unit cell, each mode being characterized by its wave vector **q**, its polarization **e** and energy E. When the number of atoms per cell is rather small (less than 10), one can easily distinguish an acoustic regime with 3 modes, where all atoms vibrate in phase at low energy, and optical excitations at higher energies.

For hypermaterials, where periodicity is absent in at least one dimension, the Bloch theorem does not hold anymore and in some sense the Brillouin zone shrinks to a point. Describing the dynamics of hypermaterials and aperiodic crystals is thus a challenging task. However, unlike amorphous systems, long range order is present in aperiodic crystals. This leads to specific signature in the dynamical spectrum. In particular, excitations specific to aperiodic crystals do appear and are named phason modes.

After a brief reminder of lattice dynamics in aperiodic crystals (1-2, 8), I will introduce simple one-dimensional systems to illustrate some of the dynamical properties of aperiodic crystals (3). A few examples in different systems will be then presented (3-7). A discussion on the implication on phase stability, thermal conductivity and thermo-dynamical properties will finally be given

References:

[1] Dove, M. T. Structure and dynamics. An atomic view of materials. (Oxford University Press, 2002).
[2] Kittel, C. Introduction to Solid State Physics.
[3] Aperiodic crystals: from modulated phases to quasicrystals, T. Janssen, G. Chapuis, M. de Boissieu, Oxford University Press 2018 (second edition)
[4] Janssen, T. & Janner, A. Aperiodic crystals and superspace concepts. Acta Cryst. B 70, 617-651 (2014)
[5] Phason modes in aperiodic crystals, de Boissieu, M., Currat, R. & Francoual, S. in Handbook of Metal Physics: Quasicrystals Advances in Metal Physics (eds T Fujiwara & Y Ishii) 107-169 (Elsevier Science, 2008).
[6] Janssen, T. & de Boissieu, M. Dynamics of quasicrystals. Comptes Rendus Physique 15, 58-69 (2014).
[7] de Boissieu, M. Phonons, Phasons and atomic dynamics in quasicrystals. Chem. Soc. Rev., 6778–6786 (2012).
[8] Useful and pedagogical simulations on simple periodic systems can be found on the Cornell SSS project web page http://pages.physics.cornell.edu/sss/