EUROPEAN SYNCHROTRON RADIATION FACILITY

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	Experiment title: Lattice dynamics of the $Al_{13}Co_4$ periodic approximant to a decagonal quasicrystal	**Experiment number:** **HC-1394**
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Repport:

Introduction The lattice dynamics of quasicrystals has been the subject of both theoretical and experimental investigations since their discovery. Because of the long range quasiperiodic order a specific dynamics can be expected. In the long wavelength regime, acoustic modes have been predicted to propagate in the (Q, E) space. For higher wave vectors, the theory predicts that the modes are critical i.e. neither extended as in simple crystals, nor localized as in disordered systems.

Many are the questions wchich remain Despite these recent advances, the nature of the modes remains an open: are the cluster playing a role? are the high Q modes critical modes ? … To tackle this problem we carry out a systematic study of phases 'approximant' of decagonal quaiscrystals. Decagonal quasicrystals are so-called 2D quasicrystals with a periodic direction and a quasiperiodic plane. This investigation will also help understanding the relationship between the structure and the vibrational properties. Experimentally, quasicrystals and approximant-crystals lattice dynamics has been studied so far by Inelastic Neutron Scattering. Unfortunately, with this technique the detection of longitudinal modes is limited to wavectors smaller than 0.2 $Å^{-1}$, because of the high sound velocity, of about 40meV/ $Å^{-1}$. For this reason we have investigated by Inelastic X ray Scattering the lattice dynamics of the approximant $Al_{13}Co_4$, (an orthorhombic phase with 102 atoms in the unit cell). This phase can be grown as a large single grain and its physical and structural properties have been fully characterized.

Experimental conditions Large single grains of about 1cm^3 have been prepared from Bridgman grown samples. A small sample of about 300µm^3 of size has been mounted in such a way to put a 'periodic' and pseudo-quaisperiodic direction in the diffracting plane. We have worked with the Si (12 12 12) and the Si (11 11 11) reflexion from the first monochromator , to get an energy resolution of 1.3 meV and a reasonnable flux. The incident energy was 23.725 keV (Si (12 12 12)) and 21.747 (Si (11 11 11)). We have measured 3 longitudinal acoustic (LA) dispersions along the periodic direction (400) to (500) and the two 'pseudo-quasiperiodic' directions (060) to (0100) and (400) to (206). Each point of the dispersion has been measured in the Energy range from -30 to +30 meV, with 4 hours/scans. The collected data have been analyzed using a Damped Harmonic Oscillator (DHO) model convoluted with the complete instrumental resolution in E and Q. A particular care has been payed to take into account the dispersion relation's slope in the convolution process. The results have been compared to atomic scale simulations carried out using adapted oscillating pair potentials.

Results and Discussion On the left, the figure shows a typical example of such a calculation for the orthorhombic phase, where a well defined gap can be seen at about 13 meV along the periodic direction. The experimental phonon spectrum shows the presence of both the acoustic and the optic modes at the crossing point (see **Fig. 3**). The transfer of intensity from the acoustic to the optic mode is a consequence of the coupling, symmetry of the structure and atomic interaction. From the phonons width we can extract the phonon lifetime: we don't observe any broadening corresponding to a lifetime reduction in correspondence of the acoustic-optic crossing. The transfer of intensity on the flat optic mode is the only important effect of this crossing, likely the key to understand the low thermal conductivity of this sample, similarly to the case of clathrates..

Along the quasiperiodic direction, no gap is observed (see **Fig. 2**).

The acoustic intensity and norm is strongly decreased along this direction. As there are several optic branches in the quasiperiodic direction, it is likely that there is a hybrization between the acoustic and the optic modes (see **Fig. 4**), which reduces the acoustic propagation, so that optic modes act as a filter.

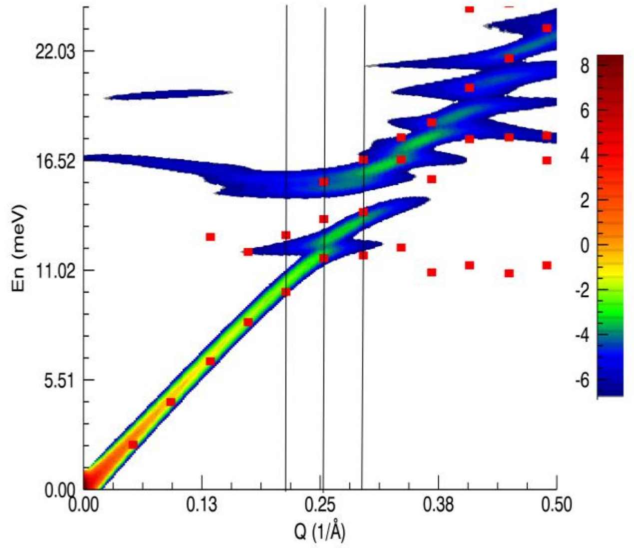

Figure 1 Phonon dispersion curve (400) to (500), with propagation along periodic direction, experiment measures (point) and simulation (continuum)

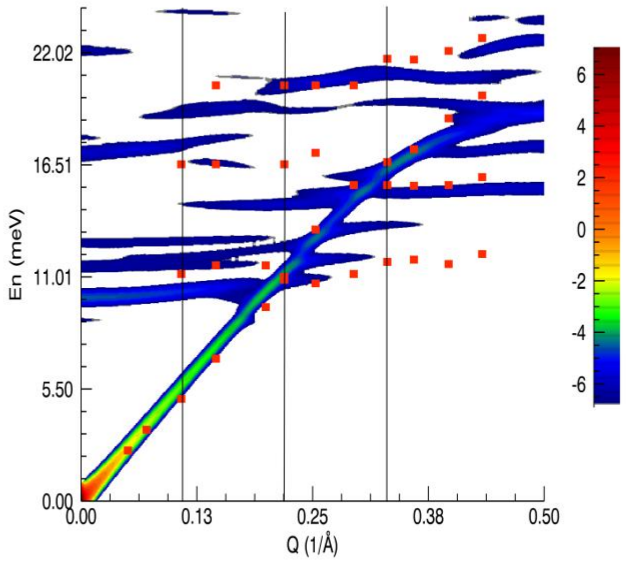

Figure 2: Phonon dispersion curve (060) to (0100), with propagation along quasiperiodic direction, experiment measures (point) and simulation (continuum)

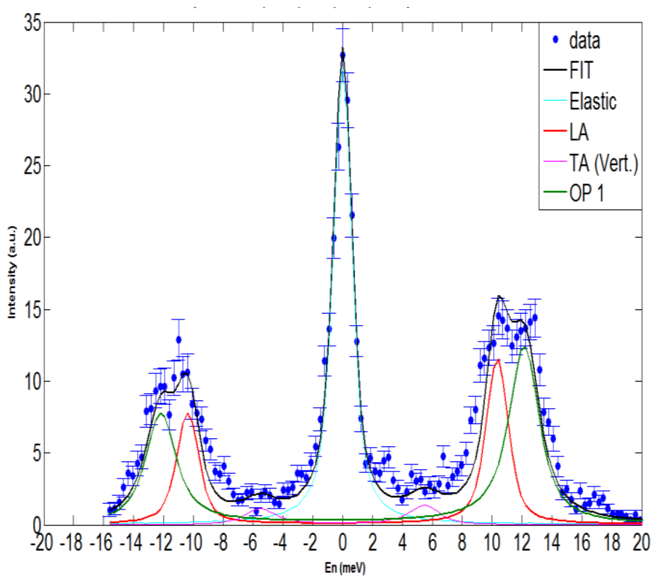

Figure 3: Phonon spectrum at **Q = 0.2526 Å^{-1}**. Coupling between the acoustic and the optic modes along periodic propagated direction

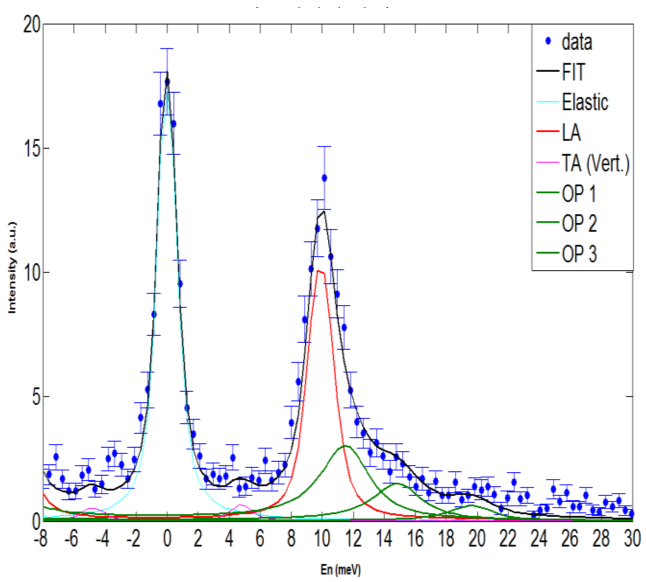

Figure 4: Acoustic phonon at **Q = 0.218 Å^{-1}**. We observe a reduction of the intensity for the acoustic mode along quasiperiodic propagated direction