Experimental Report

06/10/2013

Proposal: **TEST-2238** **Council:** 10/2012

Title: Lattice dynamics of periodic approximants to the decagonal quasicrystal

This proposal is a new proposal

Researh Area:

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Samples: Al13Co4

Instrument	Req. Days	All. Days	From	To
IN3	4	4	28/03/2013	01/04/2013

Abstract:

Experiment report: IN3 experiment Test 2238

Lattice dynamics of periodic approximants to the decagonal quasicrystal

Introduction

The lattice dynamics of quasicrystal has been the subject of both theoretical and experimental investigations since their discovery. Because of the long range, there is a quasiperiodic order hence a specific dynamics is expected. Whereas the Brillouin zone shrinks to a point, pseudo zone center and pseudo Brillouin zone can be defined. In the long wavelength regime, acoustic modes have been predicted to be best visible around strong Bragg peak, acting as zone centers. For higher wave vectors, the theory predicts that the modes are critical that to say neither they are extended as in simple crystals nor localized as in disordered systems. Experimentally, for all quasicrystals studied so far, acoustic modes have been observed around the strong Bragg peaks. The rapid acoustic mode broadening and the acoustic phonon lifetime in this area both point to a characteristic length scale of the order 10 to 20 Å, i.e. of the size of the atomic clusters that describe the atomic structure of quasicrystal.

With this experiment, we have studied the lattice dynamic of one approximants: the $Al_{13}Co_4$ phase (orthorhombic, 102 atoms in the unit cell). This compound can be grown as large single grain and its physical properties have been fully characterized [6]. The lattice thermal conductivity of the o-$Al_{13}Co_4$ anisotropy is smaller and the Umklap peak is replaced by a broad maxima.

Experiment environment

We carry out the inelastic neutron scattering on triple axis, using fixed final k_F energy equal to 2.662 $Å^{-1}$. We are used the graphic monochromator (200) and the cupper analyzer (111).

We have measured the inelastic scattering signal around strong Bragg reflection (800), this Bragg peak is in a plane containing both a ‘periodic’ and a ‘quasiperiodic’ direction (see **Fig.1**).

Discussions of the results

Beforehand, we did calculations ab-initio (DFT) on this compound. Moreover the calculations were used as assistant to define the interesting directions to measure the dispersion curves in this compound.

At first the results of this experiment are the first ones that we have obtained on this approximant o-$Al_{13}Co_4$. Then the results obtained during this experiment are very interesting. Because the measures (inelastic neutron scattering) are in agreements with the results of our calculations (DFT). For it, we have compared the dispersion curve l (800-802) between the measures and the calculations (see **Fig. 2**). On this figure, we have plotted the results from

DFT calculation (continuum plot) and the experiment results (dot line). The correspondence is perfect.

We have to find the acoustic mode cross-functional and the optical mode on the experimental measures. We have deducted the slope of the acoustic mode like 28 meV/angstrom. On the other hand we measured the gap between this acoustic mode and the optical mode at 10 meV. The value of this gap (2.23 meV) is close to it obtained in the calculations DFT.

At least the measures show the coupling between the acoustic and the optic modes in this direction. Because we find a transfer of intensity of the phonon's peak between two modes. This effect is observed at the moment where both branches are close. This remark is an experiment proof of the impact of the localised modes in the lattice dynamic in the approximant of the quasicristalline phase.

To conclude this report, these excellent results confirm the good approaches defined by the simulation (DFT). Moreover, we will continue to study this composed like the inelastic neutron scattering. And we will measure the phonon propagation along another direction.

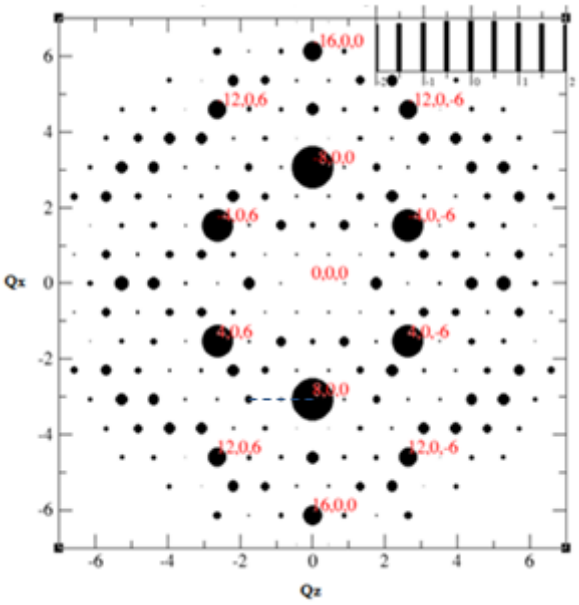

Figure 1: Diffraction pattern, plan periodic (100) and aperiodic direction (001), the dot line show the phonon propagation is measured in this experiment

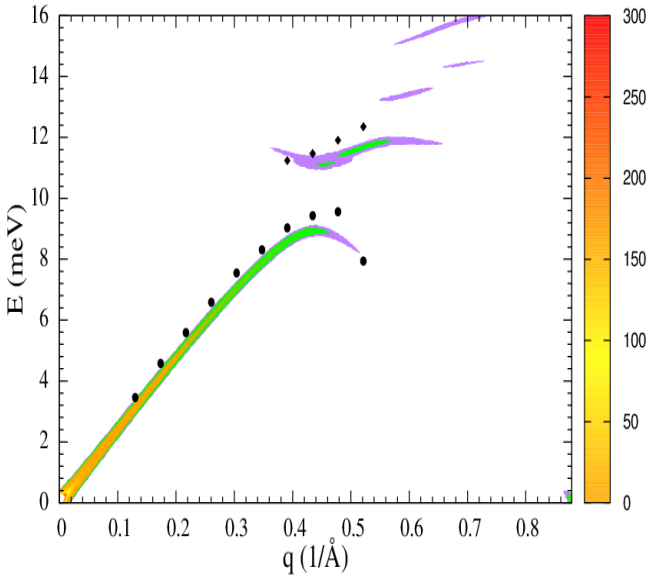

Figure 2: Dispersion curve around the Bragg peak 800 and along the direction Qz. The continuum picture is the simulation results and the dot line concerns the experiment results

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