Lattice Dynamics of the Zn-Mg-Sc Icosahedral Quasicrystal and Its 1/1 Periodic Approximant

The discovery, more than 20 years ago, of a new class of materials named quasicrystals for which atoms are arranged in a long range ordered way but without periodicity has immediately attracted the attention of mathematicians, physicists, chemists and even artists. Indeed the diffraction pattern of quasicrystals present sharp Bragg peaks, as a signature of long range order, but with symmetries, such as 5-fold rotations, incompatible with lattice periodicity (see [1] for an introduction).

The question 'where are the atoms in a quasicrystal?' could be answered only recently thanks to the discovery of the binary i-$Cd_{5.7}Yb$ icosahedral quasicrystal [2]. The quasicrystal structure has been solved using the knowledge gained from the 1/1 periodic approximant and sophisticated high dimensional analysis [3]. The atomic structure of the QC and its approximant is described by the same building block, a large atomic cluster made of 158 atoms and whose successive shell are shown Fig. 1. Clusters are connected along the 2-fold and 3-fold directions and are packed on a body centre cubic lattice in the 1/1 approximant whereas they form a quasiperiodic network in the QC as shown Fig. 1.

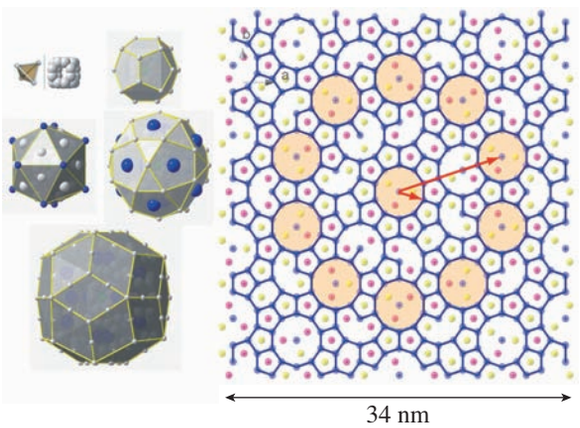

Fig. 1. Atomic structure of the CdYb quasicrystal. The left panel displays the shell decomposition of the atomic cluster. White and blue color stand for Cd and Yb atoms respectively. The cluster network in a large portion of the QC (only cluster centers are displayed) is shown in the right panel.

Understanding the effect of quasiperiodicity on physical properties remains a challenge since most solid state physics results are based on the notion of periodicity and the Bloch theorem. To tackle this problem we have studied the lattice dynamics of the Zn-Mg-Sc icosahedral QC and its 1/1 approximant. This system is isostructural to the CdYb (Zn being equivalent to Cd and Sc to Yb), with thus a detailed understanding of their atomic structure allowing simulation. Moreover the QC and 1/1 approximant allow to study the respective effect of local order (atomic clusters) and long range order (periodic or quasiperiodic) on the lattice dynamics. Within an international collaboration gathering teams from France, Japan, Slovakia, Germany and USA, the response function S(**Q**,ω) has been measured on single grain samples using X-ray (**BL35XU**, SPring-8) and neutron (LLB and ILL) inelastic scattering [4].

From the measured response function, the position, intensity and width of the observed excitation is extracted and reported on the dispersion relation shown Fig. 2 for longitudinal modes, measured on BL35XU. As for other QC, there are well defined acoustic modes in a limited q region, the signal then broaden rapidly. We also observe in both the QC and the approximant well defined dispersion-less excitation located around 6, 8, 16 meV. Besides the similarities, significant differences between the QC and its approximant have been observed. As a general trend, the 'separation' between the acoustic and optic like signal is larger in the approximant than in the QC. In some sense, the long range quasiperiodic order brings in a blurring of the S(**Q**, ω) response function. This can be understood, using the concept of quasi Brillouin zone

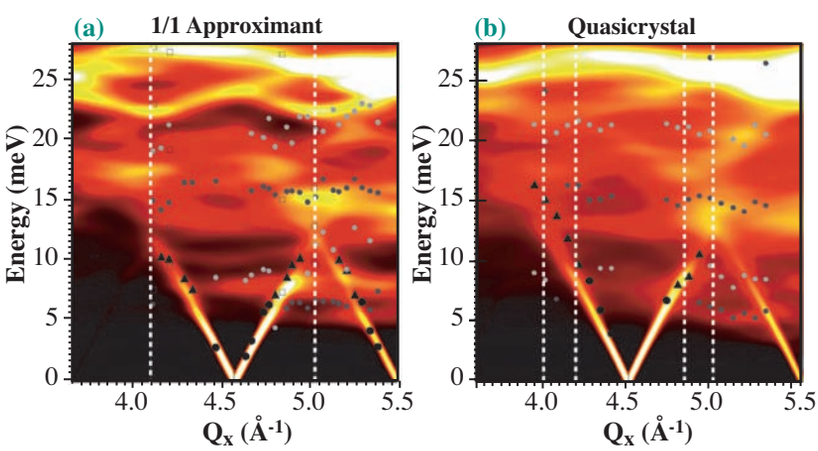

Fig. 2. Longitudinal dispersion relation measured by inelastic X-ray scattering in the approximant and the QC (symbols). The colored coded background stands for the simulation.

boundary in the QC shown as a vertical dashed line.

Those results have been compared to atomic simulations using the known structure and oscillating pair potentials for the Zn-Mg system derived from a data base of *ab initio* calculations. The quasicrystal has been simulated by a large periodic crystal containing about 3000 atoms in a unit cell and whose structure has been derived from the known QC structure. Results of the simulation, superimposed on the experimental data are shown Fig. 2. As can be seen, the simulation reproduces both the similarities and differences of the dispersion relation. The comparison has also been made on a quantitative way, which is a much stronger constraint. A few measured inelastic X-ray spectrums are compared to the simulation on the Fig. 3. The position, width and the relative intensity of the excitations are perfectly reproduced by the simulation, thus validating the model. These results open up the way for a detailed understanding of lattice dynamics of quasicrystal but also to tackle the fascinating question of why they form.

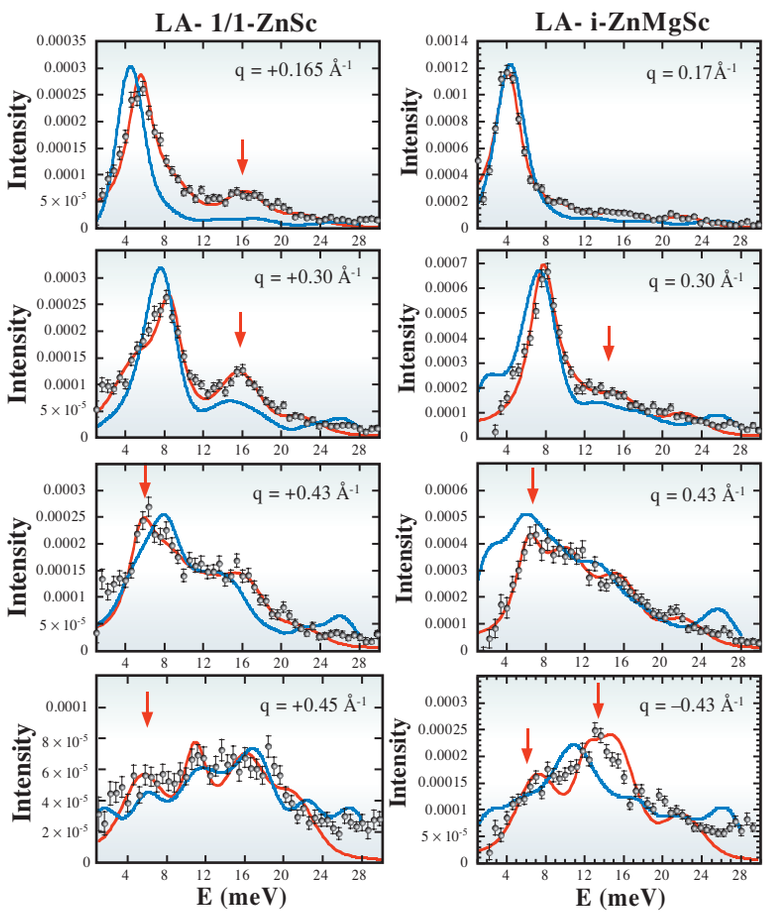

Fig. 3. Series of measured inelastic X-ray spectra in longitudinal geometry in the 1/1 approximant (left) and quasicrystal (right). The distance q from the Bragg peak or zone center is indicated in insert. The dots are for the measurements and the red line for the fit. The blue line is the simulation.

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References

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