ESRF	**Experiment title:** **Temperature dependence of phason diffuse scattering in the AgInYb icosahedral quasicrystal**	**Experiment number**: HC-876
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Report:

Quasicrystals are long range ordered materials that lack translational symmetry. Their structure is now well understood and a detailed understanding has been achieved for the icosahedral Cd-Yb phase [1] [2]. It has been shown that the CdYb quasicrystal and its approximant are built up with the same atomic cluster [3], packed on a quasiperiodic lattice or a periodic body centred cubic lattice.

One of the most fascinating questions in this field remains the mechanisms responsible for the quasiperiodic long range propagation. In this perspective two scenarii have been proposed [4]: in the first one the quasicrystal is stabilised by short/medium range order interactions leading to a quasicrystalline ground state at 0K; the second scenario point out to the importance of the entropy gained by so-called phason fluctuations. Indeed, the quasicrystalline long range order lead to suplementary diffusive like excitations named phason which are activated at high temperature. Those phason modes only exist in the quasicrystalline state, so that excess entropy is expected in the QC as compared to the periodic crystal. In this scenario, where entropy is dominating, the quasicrystal is only stable at high temperature, and transforms at low temperature through a softening of the phason elastic constants.

Phason modes give rise to a characteristic signature in the diffuse scattering intensity around Bargg peaks whos intensity distribution is determined by the two phason elastic constants K1 and K2 [5]. Temperature studies at high temperature in i-AlPdMn (between 500°C and 750°C), showed that the observed diffuse scattering intensity increases as T diminishes, a counter-intuitive observation which is in agreement with a softening of the phason elastic constant and thus support an entropy stabilisation of the quasicrystal [6].

Phason diffuse scattering has been observed at room temperature for all icosahedral quasicrystals studied so far. Recently the i-$Ag_{42}In_{42}Yb_{16}$ quasicrystal, isostructural to the CdYb one, has been synthetised in the (InAg)Yb system [8]. In this phase Ag-In replaces Cd atoms, with a vapour pressure which is much smaller, allowing thus a temperature study up to 450 C.

Large single grain of the AgInYb quasicrystal have been prepared by the Bridgman technique. The sample was placed in a furnace under secondary vacuum, and then studied under reflection geometry. An incoming beam with an energy equal to 20 keV, was used in reflection geometry to measure diffuse scattering maps

around selectred strong Bragg peaks. Systematic scans along high symmetry axis have also been carried out. A point detector was used since a high dynamical range (9 order of magnitude) is necessary to record the weak diffuse scattering close to very strong Bragg peaks.

When starting from an as-grown sample, we observe a drastic change of the diffuse scattering for temperature larger than 300C. Whereas for the as-grown sample the diffuse scattering is rather elongated along directions parallel to 5-fold axis, this is no longer the case at 350 and higher temperatuure as sjown on the figure. The diffuse scattering increases and is 3-fold elongated suggesting a negative ratio K2/K1 of the phason elastic constant. At the same time high Qper, weak Bragg peaks see their inetensity decreasing drastically: notice the much smaller number of visible weak refflection at 450 C. The transformation from 5-fold to 3-fold diffuse scattering is found to be irreversible. However, once the diffuse scattedring transformed to 3-fold like a cycle between 300 and 400 C, and experiment on a second sample seems to indicate a reversible evolution from strong to weak intensity as a function of T. However, the formation of an oxyde contamination layer, did not allow to fully confirm this. Nevertheless those results suggest that the diffuse scattering increases as T increases in agreeement with the 'energeticaly stabilized' model. Data are under evaluation, but further experiments are needed to fully confirm these observation.

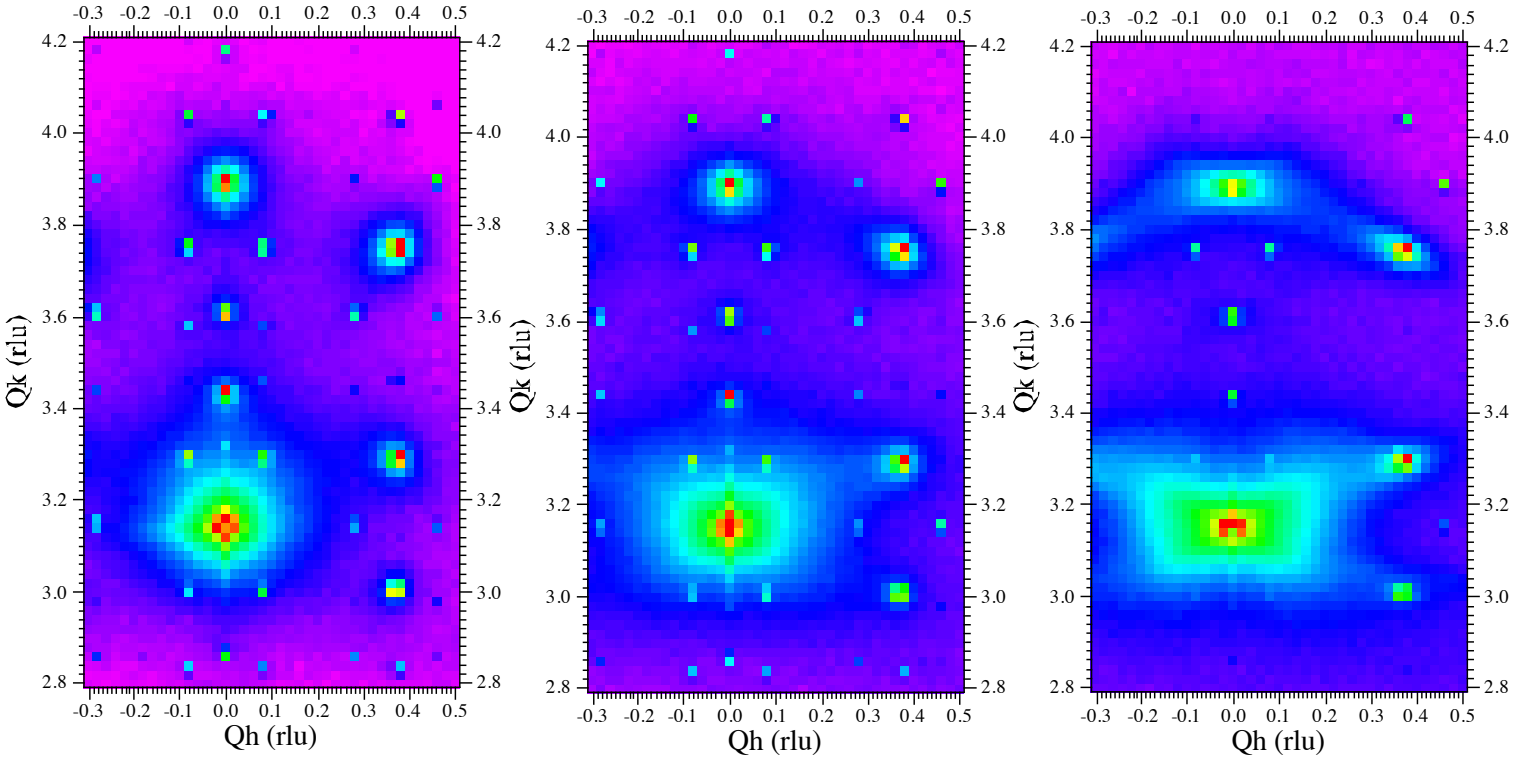

Figure: Intensity distribution of the diffuse scattering as measured in the i-AgInYb quasicrystal at room temperature (left), 350 C (middle) and 450 C (right)

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