ESRF	**Experiment title:** Temperature study of phason fluctuations in the CdYb icosahedral phase.	**Experiment number:** 02 02 632
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Report:

Quasicrystals (QCs) are long-range ordered materials which lack translational invariance. In the case of icosahedral (i-) phases, their diffraction pattern displays sharp Bragg reflections and 5-fold symmetry. Because of the quasiperiodic long-range order, there exist new modes called "phasons". Those phason modes are not propagative modes, as in incommensurately modulated structures, but collective diffusive modes. Long-wavelength phason fluctuations give rise to diffuse scattering located close to Bragg reflections in very much the same way that phonons give rise to thermal diffuse scattering (TDS). Within the elasticity theory of QCs, the diffuse scattering due to phason fluctuations can be computed and its shape anisotropy is shown to depend only on the ratio of the two phason elastic constants K2 and K1, when the phonon/phason coupling term K3 is negligible. Such 'phason' diffuse scattering has been observed in i-AlPdMn [1-2] and in the recently discovered i-$Cd_{5.7}Yb$ phase [3-4]. The phason part of the diffuse scattering is shown to dominate the whole measured diffuse scattering signal.

The i-$Cd_{5.7}Yb$ quasicrystal contains the same atomic clusters as in the Cd_6Yb crystalline approximant (Im3 space group, a=1.56 nm) whose structure is known [3]. It can be described as a body-centered cubic (bcc) stacking of a 66 atoms icosahedral cluster. The inner shell is however made of a Cd tetrahedron which one breaks the icosahedral symmetry: 4 equivalent orientations inside a cube are statistically possible for this tetrahedron. Temperature studies of the specific heat and in-situ HREM images have evidenced a phase transition taking place at 110K [5]. It has been interpreted as an order-disorder transition, where the order parameter is the inner shell tetrahedron orientation.

The purpose of the present experiment was to investigate whether such order-disorder transition is taking place in the quasicrystalline phase by performing a detailed temperature study of the diffuse scattering.

Experimental details:

The experiment has been carried out on the D2AM beamline, using the 7-circles diffractometer and at an energy of 17.9 keV. A 2-fold oriented sample i-$Cd_{85}Yb_{15}$ (2x3x1 mm^3) was extracted from a Bridgmanngrown single-grain and placed under vacuum in the displex stage equipped with a double Be hemisphere. Systematic Q-scans along the high-symmetry axis and diffuse intensity maps have been recorded at 20K, 100K, 200K and at room temperature (RT). Images of the diffuse scattering around Bragg reflections were also recorded using a 2D CCD camera.

At room temperature, all Bragg reflections could be indexed using a Pm35 primitive lattice and a 6D lattice parameter equal to 8.040 Å. As expected from previous experiments [4]. and as can be seen in fig. 1, we observe elongations of the diffuse scattering intensity along 3-fold directions from the Bragg peak. This characteristic anisotropy is a direct signature of a diffuse scattering originating from phason fluctuations. At 20K, measurements did not show any trace of supertructure reflections or anomalies in the diffuse scattering which would indicate a short-range order correlation, typical in order-disorder phase transition. We can thus conclude from the present experiment that the ordering mechanism taking place in the crystalline approximant is not occuring in the quasicrystal.

At low temperatures, the contribution from thermal diffuse scattering is much smaller. This is particularly visible around the high-Q reflections, as shown in fig.1 which displays the recorded CCD images taken at 20K (left) and 200K (right) around the 52/84 2-fold reflection. The diffuse scattering anisotropy is clearly visible at 20K, whereas it is partly masked by the TDS contribution at 200K. Further quantitative analysis of this diffuse intensity is in progress.

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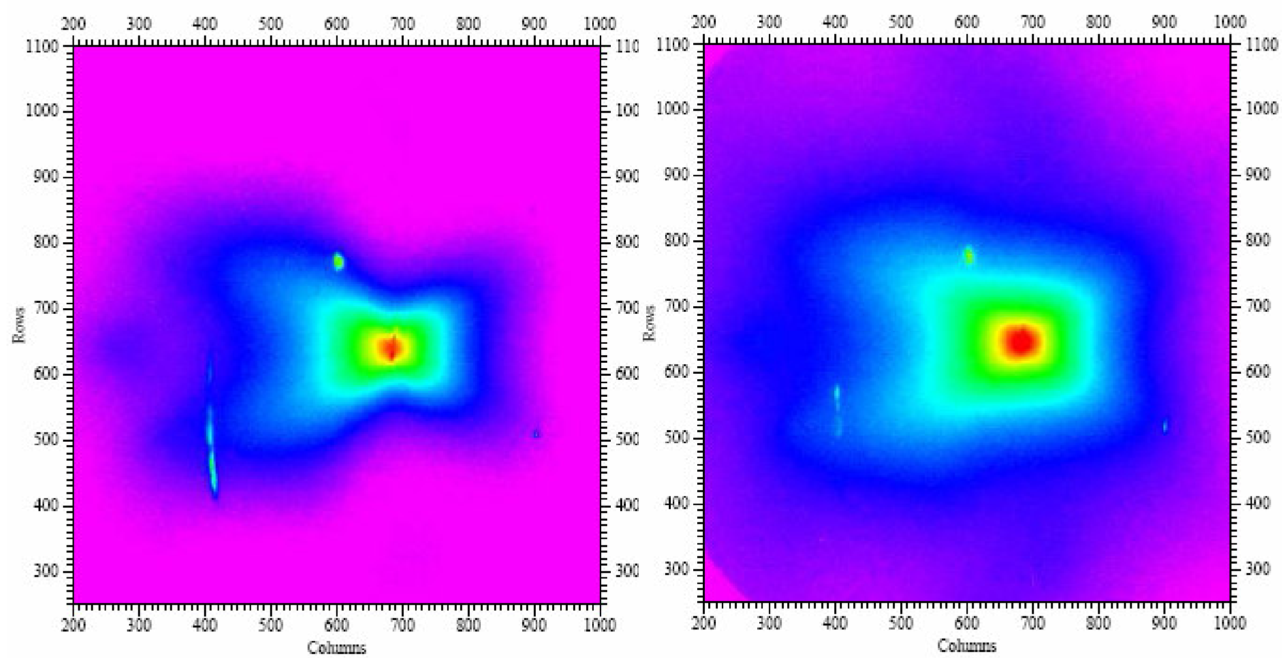

Fig. 1 : Diffuse scattering intensity measured around the strong 52/84 2-fold Bragg reflection. The sample has been set out of Bragg conditions in order to measure the weak diffuse intensity. The left and right pannels correspond to measurements carried out at 20K and 200K, respectively.

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