ESRF	**Experiment title:** Phase transition and short range ordering in the CdYb 1/1 approximant to the quasicrystal.	**Experiment number**: 02-02-820
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Report:

The discovery of the first stable binary quasicrystal in the CdYb system has been a breakthrough [1]. Indeed in this system both the icosahedral *i*-$Cd_{5.7}Yb$ and the Cd_6Yb periodic cubic approximant (*Im-3*, a=1.5 nm), having almost the same chemical composition, can be synthetised. It has been shown that the quasicrystal and its approximant are built up with the same atomic cluster (2-3), packed on a quasiperiodic lattice or a periodic body centred cubic lattice. These clusters consist of several shells, the innermost one being a Cd4 tetrahedron. Due to steric effect this central cluster induces a strong distortion of the next icosahedral shell.

The room temperature structure of Cd_6M (*M*=Ca, rare earth) and Zn_6Sc, which are isostructural to Cd_6Yb, clearly showed that the innermost tetrahedra are disordered having all the possible orientation under the cubic symmetry group [2]. At low temperature, a phase transition to a phase of lower symmetry is generally observed and corresponds to an ordering of the central Cd_4 tetrahedra (4-6).

Different ordering mechanisms have been observed so far. In the first one, which corresponds to the Zn_6Sc approximants, tetrahedra order along the [110] direction, where neighbouring tetrahedra are ordered in anti-parallel position [6-10].

The situation is different in the CdYb case for which it has been shown that both superstructure along 110 and 111 directions do occur. It was the purpose of this experiment to study this phase transition.

A single grain sample with a size approximately 1x1x1 mm was glued with silver laque on the cold finger of the newly installed cryostat. Using one module of the Xpad 2D pixel detector, we followed the evolution of the main and superstructure reflections, while cooling and heating the sample. The phase transition was observed at Tc = 106 K in very good agreement with the resistivity measurement. Below Tc we observed a Bragg peak splitting, which can be fully accounted for by a monoclinic distortion, as shown in Figure 1. The parameter found here are constituent with measurements on other 1/1 approximant, with a beta angle equal to

89.87°. The observed monoclinic distortion is essentially due to the a/c ratio being larger than one, and almost equal to b$\sqrt{2}$.

Two families of supers-structure have been observed corresponding to an ordering along 110 or 111. The ordering scheme is thus different from the Zn-Sc one. A set of 8 superstructure reflexions, belonging to the two families, has been measured between 30 and 190 K. The intensity evolution shows a smooth increase above Tc when cooling down. Both type of superstructure display the same behaviour, together with a small hysteresis. This is at variance from the previous Zn-Sc study for which the intensity showed a much more abrupt intensity increase at Tc (9). Above Tc the short range order is clearly visible, up to 50°C above Tc. The correlation length display a 'second order' divergence type, similarly to what had been observed in Zn-Sc (9). Above Tc, the correlation length is limited by the monoclinic domain size.

In conclusion, the study of the CdYb 1/1 approximant phase transition has confirmed its weak first order type, almost second order related to the central tetrahedron ordering.

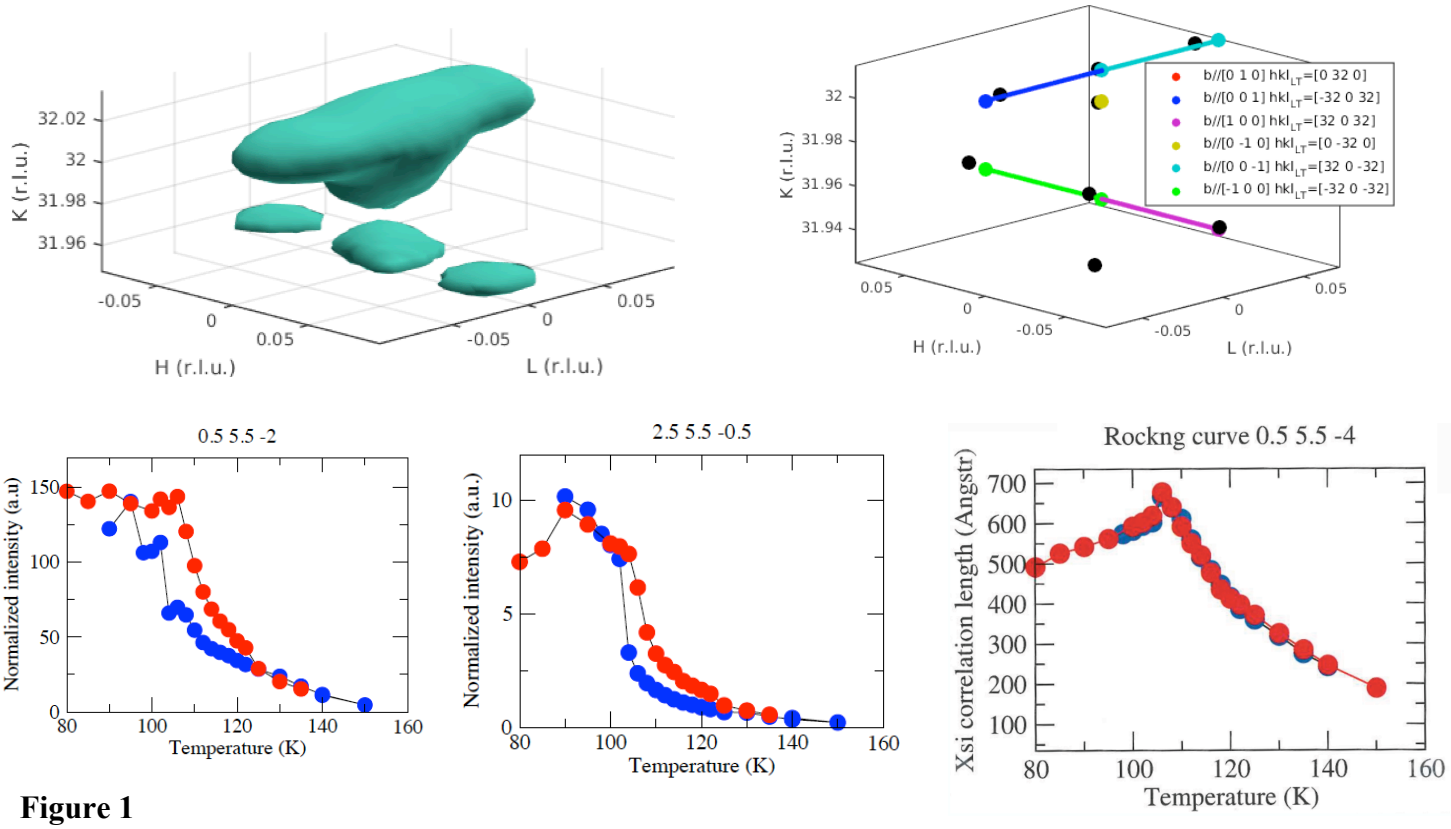

Figure 1

Top: Monoclinic distortion of the (0 32 0) Bragg peak measured at 90 K. The observation is fully accounted for by the model as shown on the right panel

Bottom: Intensity variation of the (0.5 5.5 -2) and (2.5 5.5 -0.5) super structure reflexion along (110) and (111) (left), and evolution of the correlation length as a function of the temperature. Blue and red dots stand for cooling and heating respectively.

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