ESRF	Experiment title: Short range order and diffuse scattering in the Cd6Pr 1/1 aproximant to the quasicrystal	Experiment number: 02-02-793
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Report:

Introduction

The discovery of the first stable binary quasicrystal in the CdYb system [1] has allowed a deep understanding of quasicrystal atomic structure [2]. It has been shown that both the icosahedral i-$Cd_{5.7}Yb$ and the Cd_6Yb 1/1 periodic cubic approximant (Im3, a=1.5 nm) are built up with the same atomic cluster packed respectively on a quasiperiodic lattice or a periodic body centered cubic lattice. These clusters consist of several shells, the innermost one being a tetrahedron. Due to steric effect this central cluster induces a strong distortion of the next icosahedral shell. In the cubic approximant a phase transition has been observed from a high temperature disordered state, where the tetrahedron clusters have all the possible orientation under the cubic symmetry group, towards a low temperature ordered monoclinic phase, where neighboring tetrahedron are ordered in anti-parallel position [3, 4]. In the case of the Zn_6Sc approximant, which is isostructural to the Cd_6Yb approximant [5], the structure of the low temperature phase has been determined by powder x-ray diffraction, showing the tetrahedron ordering antiparallel along the [110] direction of the HT phase and evidencing the strong distortion mentioned above [6]. The isostructure to these approximants has been found in Cd_6M (M = Ca and rare earth element).

Exprimental data and results

Large single grains of the 1/1 Cd_6Pr, $(Cd,Mg)_6Pr$ were polished with a surface perpendicular to a 2-fold axis. Systematic scan around expected diffuse scattering has been carried out between RT and 20K using incoming x-ray energy equal to 18 keV. For the Cd_6Pr sample, we observed diffuse scattering at the position of the superlattice reflection below 200 K and the diffuse intensity gradually increases as the temperature decreases to 20 K as shown in Fig. 1. In addition, any lattice distortions were found by rocking curve measurement on the 15 15 0 main reflection. These results demonstrate that the short range order of the tetrahedra is formed but not fully is ordered down to lowest temperature we measured, i.e. 20 K. The same situation was also found in the $(Cd, Mg)_6Pr$ with 10 at. % of Mg.

We changed the sample to the Cd_6Yb 1/1 cubic approximate, which is isostructure to the Cd_6Pr. We have observed Bragg and diffuse scattering below 120 K and it merges into Bragg at 90 K as shown in Fig. 2. The correlation length was estimated and found to reach ~100 nm at 90 K, which is same order we found in

Zn_6Sc (see experimental report HS-3666). On the other hand, the low-T phase of the Cd_6Yb was found to be not isostructure to the Zn_6Sc one i.e. C-centered monoclinic (Cc or C2/c). This is supported by following observations. First, any lattice distortions were found by rocking curve measurement on the 15 15 0 main reflection, indicates that the lattice is not monoclinic but cubic and the propagation direction of the tetrahedra ordering is along <111> direction of the high-T phase. Second, we observed 3 5 -1 superlattice reflection as shown in Fig. 3, which is forbidden in the above monoclinic space group also in *bcc* high-T phase. The possible ordering manner of the tetrahedral and the space group determination are underway.

In conclusion we have shown that the pre-phase transition phenomenon in Cd_6Pr and long-range ordering in Cd_6Yb. For the Cd_6Pr, short range order of the tetrahedral orientation set below to 200 K and become not fully ordered bown to 20 K. For the Cd_6Yb, the short-range order is formed below 120 K and long-range order is set at 110 K. The space group determination is underway however, present observation indicates that the the low-T structure is not isostructure to the Zn_6Sc one.

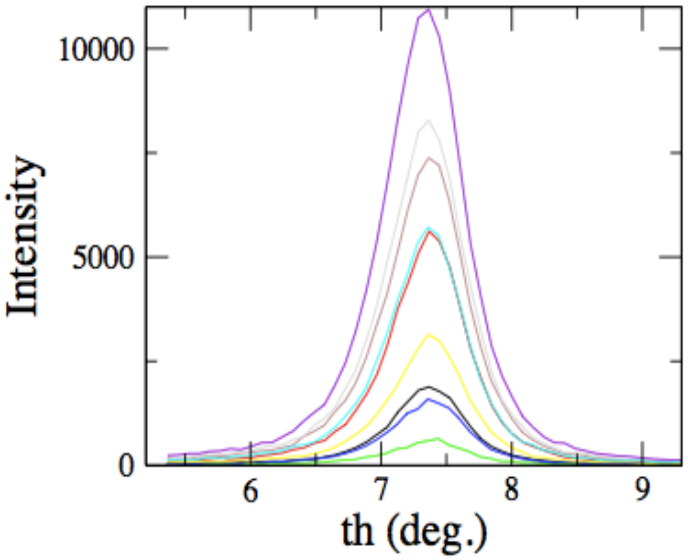

Figure 1 Temperature evolution of the diffuse scattering at the position of 0.5 5.5 2 superlattice reflection between 20 K and120 K on Cd_6Pr

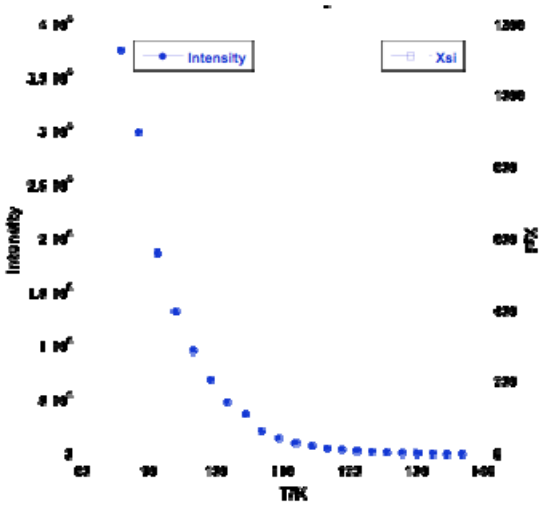

Figure 2 Temperature evolution of the diffuse intensity measured at the position of 4.5 4 0.5 superlattice reflection and the estimated correlation length between 85 K and135 K on Cd_6Yb.

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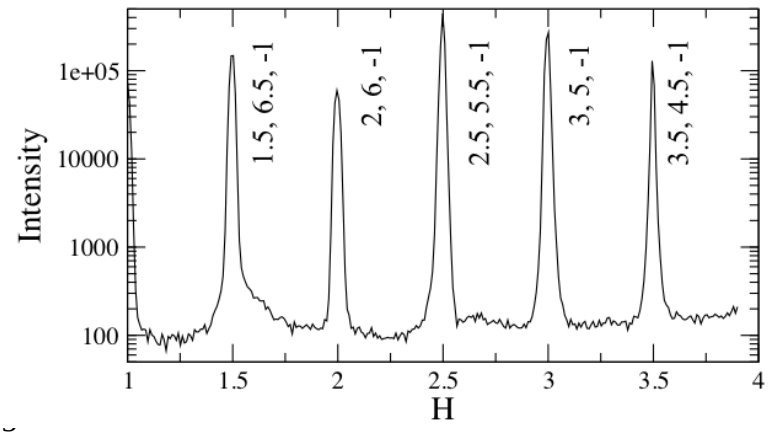

Figure 3 Line scan along [1-10] direction of the high-T phase on the Cd_6Yb at 20 K