ESRF	Experiment title: Ordering and short range order in the (AgIn)Ce and (AgIn)Eu 1/1 periodic approximant to quasicrystals.	Experiment number: 02-02-770
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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 and AgInM (M = Ca and rare earth element).

Exprimental data and results

Large single grains of the 1/1 AgInEu approximant was polished with a surface perpendicular to a 2-fold axis. Systematic scan around expected diffuse scattering has been carried out between RT and 100K using incoming x-ray energy equal to 18 keV. We did not observed any diffuse scattering and lattice distortion down to 100K, demonstrates that the sample remains with Im-3 space group. Therefore we changed the sample to the Cd_6Tb 1/1 cubic approximant which is isostructure to AgInEu and investigated diffuse scattering as well as the cubic lattice distortion.

We have observed Bragg and diffuse scattering between 150K and RT. Bellow Tc ~165K, a phase transition occurred with a peak splitting and superstructure reflections along the [110] direction. The low-T phase is most likely isostructure to the Zn6Sc one. The lattice distortion has been evidenced by peak split of the (15 15 0) main reflection measured between 160K and 170K as shown in figure 1.

Above Tc, broad diffuse scattering was observed at the positions of superlattice reflection at 230K and found to be merged into a Bragg at the lattice distortion temperature, saying that the short-range order exists and developed with decreasing the temperature. The correlation length reaches ~1000 Å with decreasing the temperature following a power low or a liner dependence (figure 2). The results thus have some similarities with Zn_6Sc approximant (see experimental report HS-3666), At 210K we measured diffuse scattering along both longitudinal and transverse directions with high resolution scans and observed the short-range order is anisotropic.

In conclusion we have shown that the phase transition in Cd_6Tb is similar to the Zn_6Sc. Short range order of the tetrahedral orientation sets in above Tc. A lattice distortion and a sharp transition occurs before the full divergence of the correlation length, although the long range order is already ~1000 Å, i.e. quite large, at the phase transition.

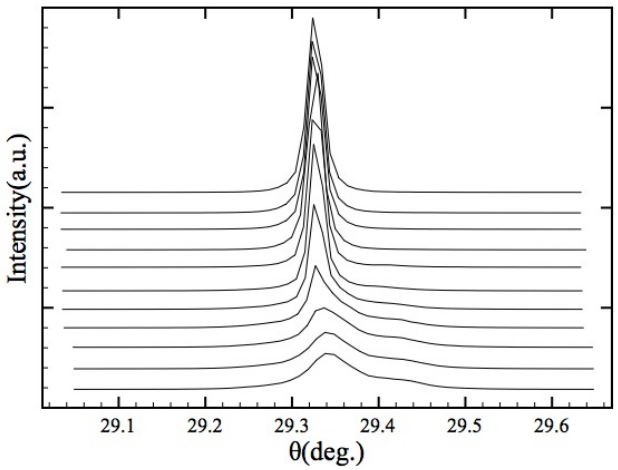

Figure 1: Peak profiles of (15 15 0) main reflection between 160K and 170K.

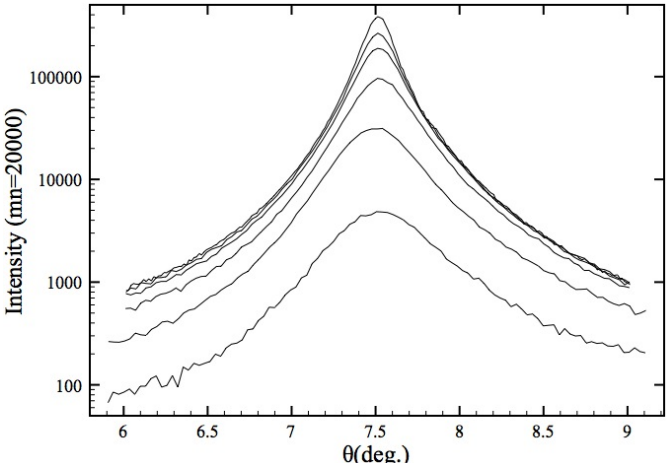

Figure 2: Diffuse scattering profile observed at the position of the 0.5 5.5 2 superlattice (int. log scale).

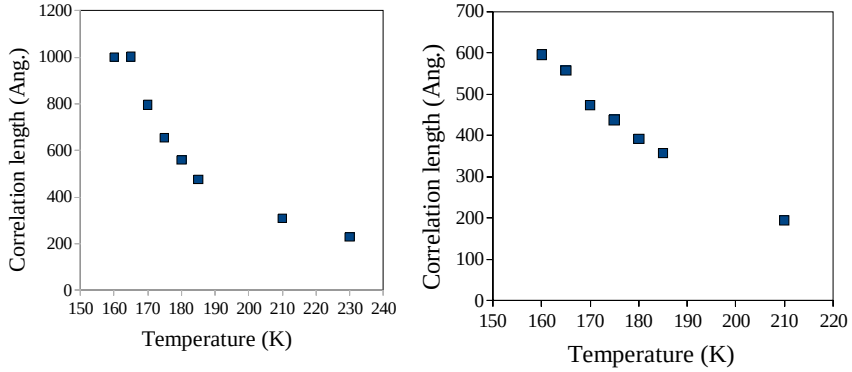

Figure 3: Temperature dependences of the correlation length. The dependences on the left and right were estimated the diffuse scattering at 0.5 5.5 2 and 5.5 4 -0.5 superlattice positions, respectively.

References

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