ESRF	**Experiment title:** Pressure and temperature phase diagram of the Zn6Sc 1/1 approximant to the quasicrystal.	**Experiment number**: HS4712
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Report:

Introduction

Quasicrystals are materials with long range order but without the lattice translation symmetry. Their atomic structure is now better understood thanks to the discovery of the binary icosahedral phase *i*-$YbCd_{5.7}$ in 2000 [1] which led to a detailed understanding of the atomic structure of the CdYb icosahedral phase [2]. Both the quasicrystal and its periodic approximant of cubic symmetry can be described by a quasiperiodic or periodic packing of the same atomic cluster which is made of successive shells of approximate icosahedral symmetry and contains 158 atoms. One characteristic feature of this cluster is the central Cd tetrahedron, which breaks the icosahedral symmetry of the other shells (Figure 1). It has been shown that the tetrahedron is orientally disordered in the cubic $YbCd_6$ approximant at room temperature [3] and orders below 110K, leading to a phase of lower symmetry [4]. It is believed that this central tetrahedron plays a crucial role in stabilizing the quasicrystalline long range order, it is therefore important to understand the detailed ordering mechanism and the nature of the interactions leading to this ordering.

Watanuki et al. have investigated the phase stability of the $YbCd_6$ approximant in the temperature-pressure regime up to 5.2 GPa and down to 10K. They have observed an extremely rich structure with up to five different superstructures. In particular the direction along which the ordering develops is pressure dependent (either 110 or 111). Moreover, T_c increases when the pressure increases [7].

Isostructural phases have been discovered in the Sc-Zn system were the quasicrystal ZnSc and the 1/1 approximant Zn_6Sc have been synthesized [5-6]. The 1/1 cubic approximant $ScZn_6$, also displays a low temperature phase transition. The structure of the low-temperature phase has been determined by synchrotron powder X-ray diffraction, showing that the Zn tetrahedra are ordered in an antiparallel fashion along the [110] direction of the high- temperature phase [6]. It is postulated that one main driving force of the phase transition is the close-packing of Zn and Sc atoms.

Recently, we obtained a millimeter size single grained $ScZn_6$ which shows a sharp phase transition at about 160K, clearly evidenced on synchrotron experiment (D2AM beam line). The purpose of the experiment was a study of the P,T phase diagram of this Zn_6Sc periodic approximant..

Exprimental data and results

Small single grains were obtained by crashing a millimeter size single grain. The single grains were mounted inside a diamond anvil cell and inserted in a low temperature helium flow cryostat for P and T studies. X-ray diffraction measurements were carried out with theta-scan between -30 and 30 degree with a 0.5 degree step at various P and T.

Firstly, we increased the pressure from 18 to 35 GPa at room temperature and correct diffraction images at some pressure (18, 24, 30, 34 and 35 GPa). Figure 3a shows a reflection observed at 30 GPa, represented in reciprocal space. The obtained superstructure reflections correspond to 4 times super cell. The diffraction pattern is found to correspond to the phase C in figure 2, which was observed in the previous experiment (see experimental report: HS4712). Next we investigated a transition pressure between phase C and bcc phase. Pressure was decreased from 35 to 0.3 GPa and the measurements were carried out with about 2 GPa step, and we observed the transformation from phase C to bcc HT phase at 20 GPa.

To investigate a transition pressure between phase A and phase B, we carried out data collection at pressures from ambient to 25 GPa at a constant temperature equal to 150 K. We observed the transformation form phase A to B when P increase from 7.5 to 7.6 GPa .

In the present experiment we could determine some borders of P-T phase diagram and collected data sets for structure determination for new superstructures. The solving atomic structures of phase B and C is in progress.

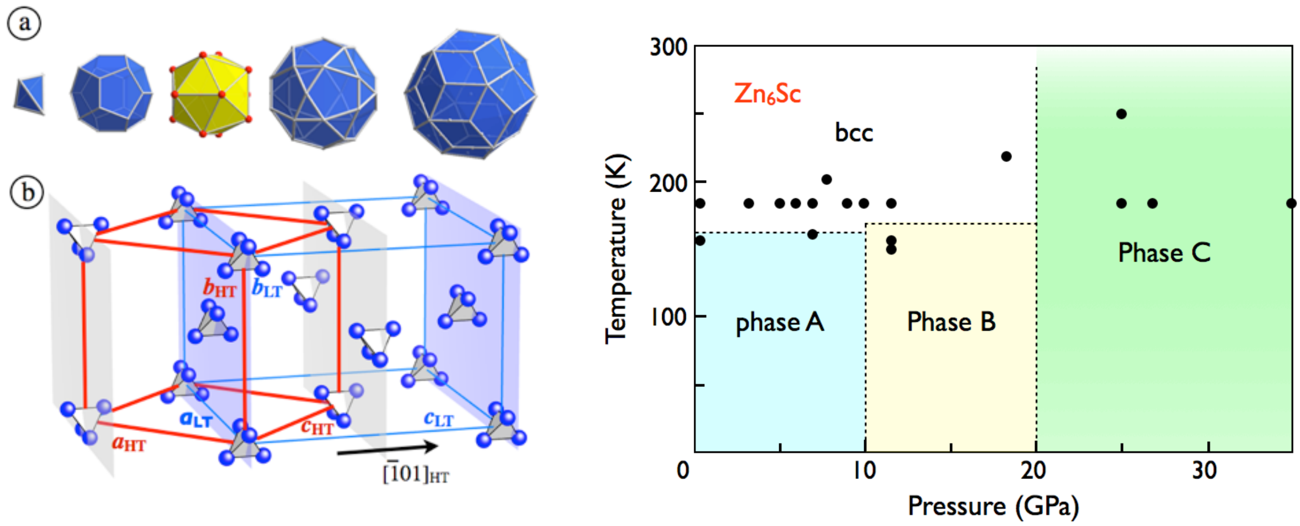

Figure 1: Left: Illustration of the phase transition showing the tetrahedron ordering. Right Schematic P,T phase diagram of the Zn6Sc phase.

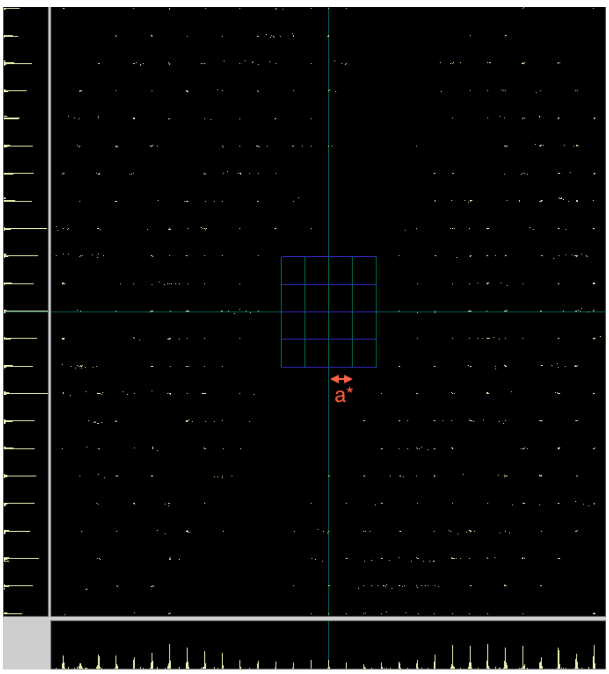

Figure 2: Reflection observed at 30 GPa at room temperature, represented in reciprocal space. Superstructure reflections corresponds to the 4 times larger superstructure can be noticed on the lower panel.

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