	Experiment title:	Experiment number:
ESRF	Diffuse scattering and phason modes in the $Zn_{88}Sc_{12}$ icosahedral quasicrystal.	02-02-766
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Report:

Introduction

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*-Cd5.7Yb and the Cd6Yb periodic cubic approximant, having almost the same chemical composition, can be synthesized. It has been shown that the quasicrystal and its approximant are built up with the same atomic cluster [2], packed on a quasi-periodic lattice or a periodic body centered cubic lattice. This knowledge together with a data collection carried out on the D2AM beamline of the ESRF and a 6D approach leads to the first accurate atomic model of a quasicrystal [3].

The recently discovered icosahedral quasicrystal $Zn_{88}Sc_{12}$ phase [9] is isostructural to the *i*-Cd5.7Yb, where Zn and Sc substitutes for the Cd and Yb atoms, respectively. Millimeter size single grains can be obtained in this system, and the purpose of the experiment was the study of phason diffuse scattering [5]. Indeed the aperiodic long range order brings in new long wavelength excitations named phasons. As for the phonon, phason modes give rise to phason diffuse scattering located nearby the Bragg peaks and with a characteristic shape [5]. It has been evidenced in the AlPdMn quasicrystal [6] and in the ZnMgSc quasicrystal [7].

Exprimental data and results

Millimeter size single grains of the $Zn_{88}Sc_{12}$ quasicrystal were polished with a surface perpendicular to 5-fold axis. Diffuse scattering has been measured for both non-annealed and annealed (at 200° C for 3 weeks) samples using an incoming x-ray energy equal to 9.3 keV. Systematic Q-scans along the high symmetry axes could be indexed with a primitive icosahedral lattice as shown on the figure 1 which displays a scan along a 2-fold axis. The maximal Q_{perp} value necessary for indexing has been found to be less than 3, i.e. much smaller than for ZnMgSc quasicrystals where the maximum value was 7 [7]. As a result very few weak reflections are visible. Annealing the sample only led to a slight improvement of the quasicrystal quality, as seen from Fig.1, where a reflection having high Q_{perp} component is clearly observed in the annealed sample.

For both the annealed and un-annealed sample we found a significant broadening of the Bragg peaks with an almost linear Qperp dependence, as a signature of a linear phason strain distribution (Figure 2). The slope is equal to ~ 5×10^{-3}, i.e. 10 times larger than the best known quasicrystal so far [8].

A large and characteristic distribution of diffuse scattering is observed on both samples as shown on the 2D map, figure 3. This diffuse scattering is due to long wavelength phason fluctuations. The determination of the phason elastic constant is underway but the elongation of the diffuse scattering along directions parallel to a 3-fold axis points towards a negativeK2/K1 ratio.

In conclusion we have shown that the newly discovered $Zn_{88}Sc_{12}$ quasicrystal contains a lot of both linear phason strain disorder and phason diffuse scattering resulting in a lower quality than the Zn-Mg-Sc quasicrystal. The crystal quality is found to be slightly improved by low-temperature long-time annealing.

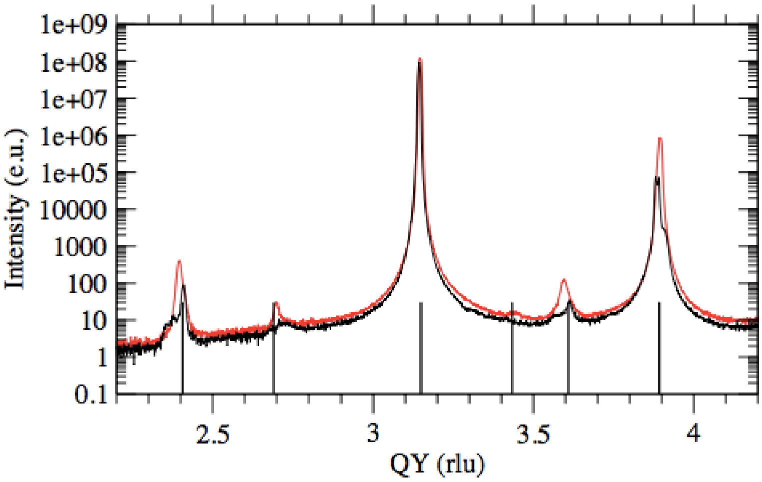

Figure 1: Comparison of the 2-fold Q-scans measured for the i-ZnSc quasicrystal, non-annealed (black) and annealed (red)

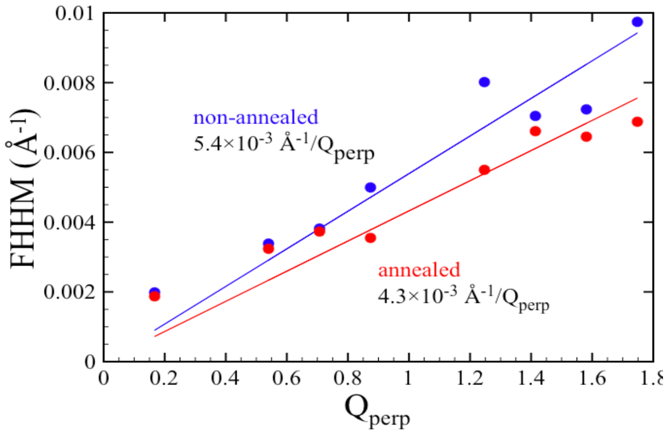

Figure 2: Qperp dependence of the FWHM for peaks measured along 5-fold axis

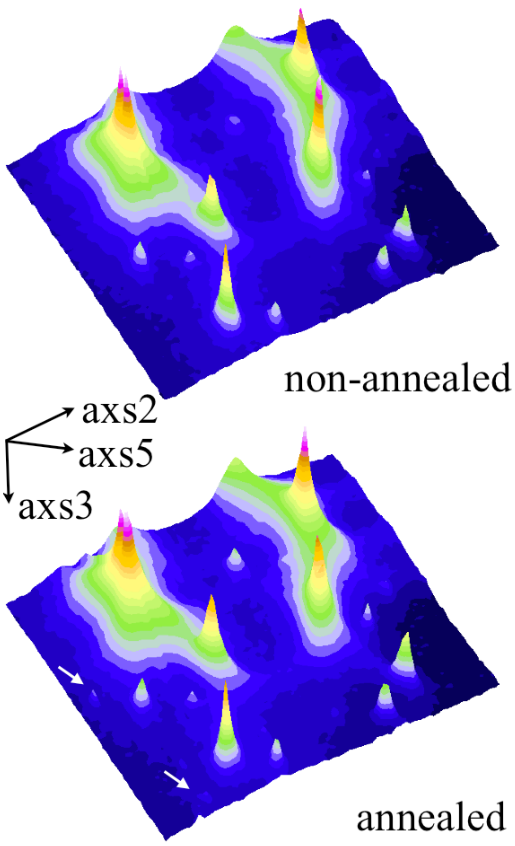

Figure 2: Diffuse scattering measured around 2- and 5-fold reflections on a HK0 plane in non-annealed (top) and annealed (bottom) samples of ZnSc quasicrystal. Strong diffuse scattering are visible along 3-fold axis in both samples, and reflections having high Q_{perp} component are observed only for the annealed sample as indicated by arrows.

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