ESRF	**Experiment title:** Icosahedral quasicrystal symmetry measured using dynamical diffraction	**Experiment number**: 02-02-832
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Report:

Quasicrystals are fascinating materials, which are long range ordered but lack translational symmetry (see 1 for an introduction). Since their discovery, numerous experiments have confirmed that for the best samples, obtained by slow cooling from the melt, Bragg peaks are extremely sharp, limited by the instrumental resolution [1; 2]. Dynamical diffraction, a signature of a very good long-range order, has also been observed [3].

For icosahedral quasicrystals, high resolution x-ray diffraction has been carried out at synchrotron, and weak departure from the icosahedral symmetry has, in some cases, been observed [4]. Icosahedral quasicrystals are indexed using a 6 dimensional cubic reciprocal lattice (6 integer indices). The 6D reciprocal vector is the sum of the physical space component (3D) and the so-called perpendicular or phason component (3D). Any departure from the perfect icosahedral symmetry can be expressed in term of a strain of the 6D lattice along the 'phason' component, using a so-called phason strain matrix, which for particular coefficients lead to a periodic approximant. In high resolution x-ray measurement along a given symmetry direction, this shows up as a deviation from the ideal position dQ which is proportional to the Q_{per} or phason component of the reciprocal wave vector as shown figure 1. The accuracy of this measurement is limited by the instrumental resolution on one hand and the largest Qper component that can be measured (large Q_{per} Bragg peak are extremely weak, since the intensity decays roughly as $Qper^{-6}$). As a consequence, the accuracy in determining the phason strain matrix which can be obtained in this case correspond to periodic approximant detection of the order 7 nm.

Recently, a new method has been proposed for such measurement. Using dynamical diffraction an extremely high high accuracy of the measurement of the phason strain matrix can be achieved, as it is the case when interferences are at play (here double diffraction). In this measurement a so called psi-scan (azimuthal scan) is carried out with a single grain quasicrystal, on a relatively weak Bragg peak. When rotating the crystal, well visible Reninger peaks are visible.

Using this approach we have undertaken psi-scan measurements on the D2AM beam line and using two samples: the i-AlPdMn and the i-ZnSc. Whereas no phason strain has been previously evidenced in the i-AlPdMn case a small component was observed in the i-Zn-Sc one.

We measured psi-scan for 3 different reflexions in each of the 2 samples.

A typical portion of the psi-scan as obtained for a 5-fold axis Bragg peaks in the Zn-Sc icosahedral quasicrystal is shown in Figure 1. It is compared with a calculation, taking a-into account all the possible multiple scattering using the known UB-Matrix and the list of measured intensities (). As can been seen the overall agreement is rather good.

However, with respect to the calculated pattern, made under the assumption of perfect icosahedral symmetry, there are clear peak shifts related to the phason distortion. Since both ‘positive’ and ‘negative’ shifts are observed, we can rule out systematic errors.

The extraction of the phason strain matrix from these data is under current evaluation.

For a better comparison we also measured accurately using the 2-D detector the reciprocal position of about 10 Bragg peaks of the icosahedral Zn-Sc quasicrystal. Peak shifts were easily visible, and an approximate phason strain matrix has been extracted.

We will use this phason strain matrix as an input and refined it against the experimental data.

This ‘proof of principle’ experiment is thus successful. The influence of the UB matrix accuracy and/or sample/goniometer alignement needs to be carried out .

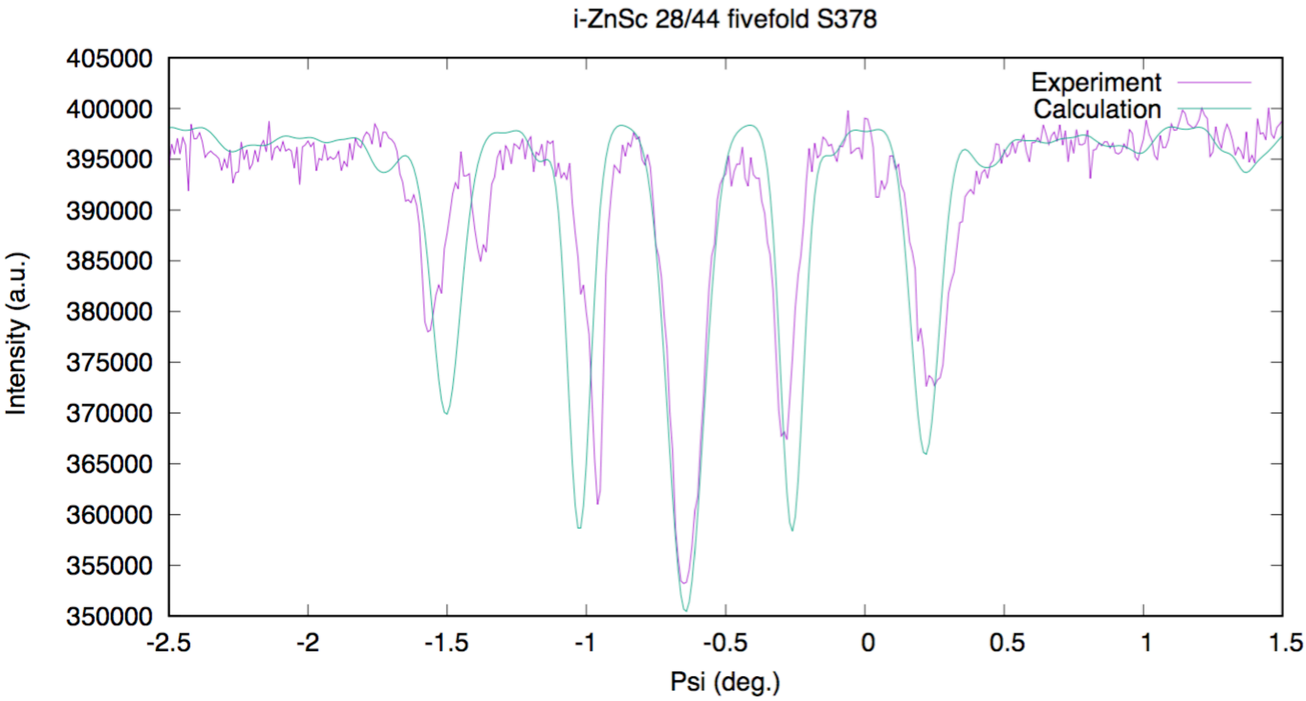

Figure 1: Psi-scan as measured in a restricted Psi region for the 28/44 5-fold Bragg peaks of the i-ZnSc quasicrystal. Reninger peaks are seen as intensity decrease in the scan (violet line) the solid line is the simulation assuming a perfect icosahedral symmetry.

References

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