ESRF	**Experiment title:** **Temperature dependence of phason diffuse scattering in the AgInYb icosahedral quasicrystal**	**Experiment number**: 02-02 816
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Report:

Quasicrystals are long range ordered materials that lack translational symmetry. Their structure is now well understood and a detailed understanding has been achieved for the icosahedral Cd-Yb phase [1 2]. It has been shown that the CdYb quasicrystal and its approximant are built up with the same atomic cluster [3], packed on a quasiperiodic lattice or a periodic body centred cubic lattice.

One of the most fascinating questions in this field remains the mechanisms responsible for the quasiperiodic long range propagation. In this perspective two scenarii have been proposed [4]: in the first one the quasicrystal is stabilised by short/medium range order interactions leading to a quasicrystalline ground state at 0K; the second scenario point out to the importance of the entropy gained by so-called phason fluctuations. Indeed, the quasicrystalline long range order lead to suplementary diffusive like excitations named phason which are activated at high temperature. Those phason modes only exist in the quasicrystalline state, so that excess entropy is expected in the QC as compared to the periodic crystal. In this scenario, where entropy is dominating, the quasicrystal is only stable at high temperature, and transforms at low temperature through a softening of the phason elastic constants.

Phason modes give rise to a characteristic signature in the diffuse scattering intensity around Bargg peaks whos intensity distribution is determined by the two phason elastic constants K1 and K2 [5]. Temperature studies at high temperature in i-AlPdMn (between 500°C and 750°C), showed that the observed diffuse scattering intensity increases as T diminishes, a counter-intuitive observation which is in agreement with a softening of the phason elastic constant and thus support an entropy stabilisation of the quasicrystal [6].

Phason diffuse scattering has been observed at room temperature for all icosahedral quasicrystals studied so far. Recently the i-$Ag_{42}In_{42}Yb_{16}$ quasicrystal, isostructural to the CdYb one, has been synthetised in the (InAg)Yb system [8]. In this phase Ag-In replaces Cd atoms, with a vapour pressure which is much smaller, allowing thus a temperature study up to 450 C.

In a previous experiment, we observed a significant change in diffuse scattering for temperature larger than 400°C, however with a surface oxydation (mainly Yb oxydation) (expt report . We have carried out a similar experiment

Large single grain of the AgInYb quasicrystal have been prepared by the Bridgman technique. The sample was placed in a furnace under a N2 flow, and then studied under reflection geometry. An incoming beam with an energy equal to 20 keV, was used in reflection geometry to measure diffuse scattering maps around selectred strong Bragg peaks. Systematic scans along high symmetry axis have also been carried out. A point detector was used since a high dynamical range (9 order of magnitude) is necessary to record the weak diffuse scattering close to very strong Bragg peaks.

Similarly to the previous experiment we observed a large change in the diffuse scatering for T larger than 300°C. The heat traeted sample was then rapidly analysed by SEM and repolished. The SEM analysis confirmed the formation of an oxyde layer, whereas the repolished sample did show a diffuse scattering intensity distribution similar to the 'fresh' sample, demonstrating that the change in diffuse scattering is the result of the oxyde/quasicrystal interface strain.

The rapid Yb oxydation, despite either a good secondary vacuum, or a N2 flow, prevented thus to carry out a quantitative measurement of the diffuse scatering intensity as a function of T. It showed nevertheless the very strong influence an interface can have on the diffuse scattring distribution and its relation to phason fluctuations. An interpretation of such a result remains a chalenging open question.

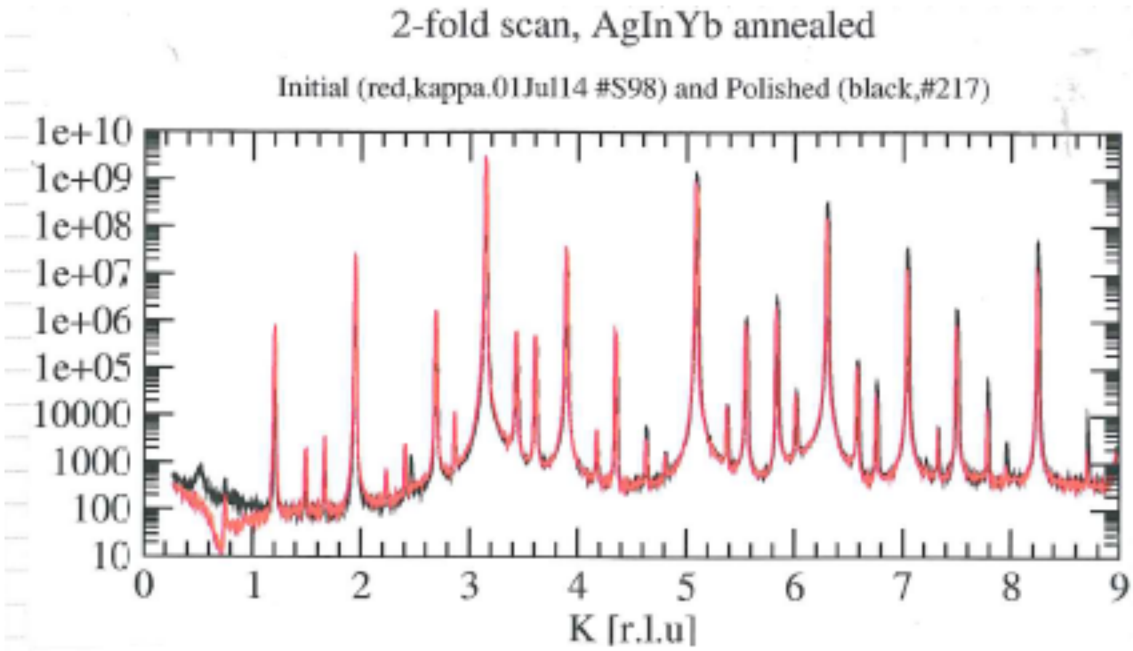

Figure: 2-fold scans measured after heat treatment and repolishing (red curve) and for the initial 'fresh' sample (black) There are no differences. The same is true for the diffuse scattering profiles.

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