ESRF	**Experiment title:** **Inhomogeneities, structural defects and growth in quasicrystals investigated by in-situ and real time X-ray diffraction, absorption and phase imaging**	**Experiment number**: HS-1030
Beamline: ID19	**Date of experiment**: from: 15.02.00 to: 3.11.00	**Date of report**: 21.02.01
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Report:

This report deals with experiments carried out during the beam time allocated in the first half of the second year of a long-term project. The aim of this project is to better understand defects previously observed in icosahedral AlPdMn quasicrystals [1-4].

Quasicrystals are solids that present long range atomic order but no periodicity. Their highly complex structures result in peculiar physical properties like a high electric resistivity although the quasicrystal contains only atoms that form metals in their elementary states. In the recent years the measurements of the properties have become more and more precise. At this stage, defects are believed to have a great impact on these measurements. The defects studied in this project are pores and defects that give rise to loop-shaped contrasts in X-ray topography. The pores were examined by phase sensitive radiography in a large variety of icosahedral AlPdMn samples in order to determine their origin. During this work we discovered that the experiments proposed in the long term project could not be interpreted without a more fundamental study of the contrast formation mechanisms in synchrotron radiation topography. Therefore, a systematic study of the defect contrasts was carried out. The effect of lattice deformations due to the defects on the structural perfection was also studied by anomalous transmission.

Systematic study of typical defect contrasts

This part of the project is a fundamental study of contrast formation in synchrotron radiation topography. It was necessary prior to the interpretation of the defect contrasts observed in the quasicrystals. The results obtained have given rise to a publication [6]:

Article title : '***The Variation of Quasicrystal Defect Contrast: How and Why***'

Abstract: '*We carried out a systematic study of typical defect contrasts in various single grains of icosahedral Al-Pd-Mn quasicrystals. White beam topographs with different sample-to-detector distances and multiple crystal topographs with different sample-to-detector distances, different working points on the rocking curve and different harmonic reflections have been recorded. Despite the extreme geometrical resolution at the ID19 topography beamline of the ESRF white beam topography showed reasonable (not blurred) contrast only for very short sample-to-detector distances (< 4 cm). Depending on the defect type, in synchrotron multiple crystal topography the defect contrast changes considerably as a function of the position of the working point on the rocking curve. Under the special conditions chosen, the dependence of contrast shape and size on the harmonic reflection used was rather weak.*'

Structural perfection and anomalous transmission

The influence of defects in quasicrystals on another measure of crystal perfection, anomalous transmission or Borrmann effect, was also studied. It was shown that the Borrmann effect could also be observed in a non-periodic structure. The results have been published [7]:

Article title: ***'Anomalous Transmission of X-rays in Quasicrystals'***

Abstract: *'The perfection of one of the quasicrystal grains with the highest degrees of perfection was checked by means of X-ray diffractometry and X-ray topography. Full widths at half maximum of de-convoluted reflectivity curves were close to the theoretical values and a partial Borrmann effect was clearly visible in the measured reflection and transmission curves, whereas the topographs showed still rather strong intricate contrast, what means that strong deformations (defects) still exist in the grain. Consequently, dynamical effects like anomalous transmission were confirmed to exist in selected quasicrystalline grains, but even then the structural quality is still far from being "highly perfect".'*

Porosity

Pores were observed in icosahedral AlPdMn samples, but their origin is still not understood. First studies of the volume fraction of the pores and their sizes as functions of the chemical composition and growth parameters provided interesting clues, which require to measure accurately the size of the pores. To carry out such a purpose, phase sensitive radiographs of pores, termed 'pore images' hereafter, were recorded. However, the sizes of the pore images are not equal to the sizes of the pores themselves. This is due to the fact that a pore in a material acts as a converging lens for X-rays, the focal length depending on the diameter of the pore and the energy of the X-rays. As a consequence and even at a fixed energy, the size of an individual pore image depends on the sample to detector distance. In order to retrieve the true pore sizes from their images we have performed numerical simulations of images corresponding to pores of the same shape and size. The detection of the smallest pores (diameters of 1 to 3 μm) was very difficult from single images. We have therefore recorded images of the pores using different sample to detector distances. This procedure allows reconstructing the spatial distribution on the exit surface of the sample of the phase shifts introduced by the pores [5] (fig. 1). This has already proven to be clearly more efficient for the detection of the smallest pores and the determination of their sizes. The exploitation of these data is in progress. The results will be submitted for publication.

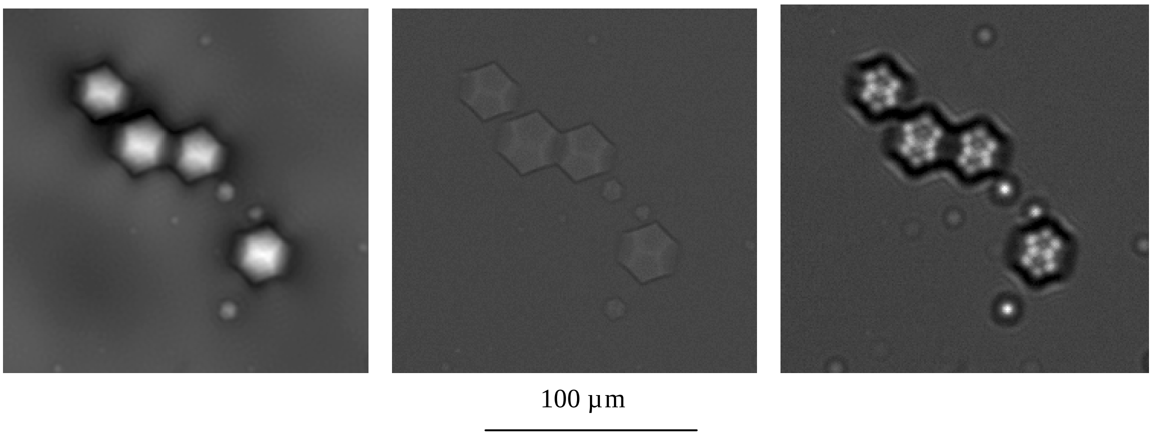

Fig.1. Phase contrast images of pores recorded at 10 and 50 cm (left, centre). These images show the variation of the contrast and the size of the pore images with the increasing distance. The pores are oriented with a two-fold axis parallel to the X-ray beam. Holographic reconstruction of the same region by images recorded at 1, 10, 20 and 50cm (right). This image reproduces the true shapes and sizes of the pores.

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