ESRF	**Investigation of the structural perfection of quasicrystals by a combination of high resolution X-ray diffraction, X-ray diffraction imaging and phase sensitive radiography**	**Experiment number**: HS-2091
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Report:

Quasicrystals are solids that present long-range atomic order but no periodicity. The most striking consequence of this is the possibility to observe 'non-crystallographic' rotational symmetries, e.g. 5- or 10-fold symmetry axes. The highly complex structures of quasicrystals result in peculiar physical properties like e.g. a high electric resistivity although the quasicrystal contains only atoms that form metals in their elementary states.

In the recent years researchers have obtained quasicrystals of rather high quality showing rocking curve widths comparable to those of the best metallic crystals. The physical properties of quasicrystals have been measured more and more precisely, which has promoted the understanding of these intriguing materials. At this stage, defects are believed to have a great impact on the physical properties. However, despite the big effort undertaken in the last years, especially on icosahedral Al-Pd-Mn, Al-Cu-Fe and Zn-Mg-RE (RE-Rare Earth) alloys grown by slow solidification techniques, the defect formation, the exact strain field around them, including the extent of the strain field in each of its subspaces (phonon and phason strain), and the way these defects can move, are far from being fully understood. Concerning the quasicrystal growth, the activities are going on two directions, firstly, to improvement of the growth methods, secondly, to synthesise new systems and phases. Recently Tsai and co-workers discovered a new class of icosahedral phases in the binary CdYb system [1, 2]. This new phase has an atomic structure completely different from the one already known in the i-Al-Pd-Mn system. Millimetre-sized quasicrystal single grains, whose atomic structure is similar to the one of the binary CdYb phase, can be obtained in the new Zn-Mg-Sc icosahedral ternary alloy [3].

In this present work we started to study the perfection, and in advantageous cases also the defects, in those new phases with the intention to compare them to our previous results obtained on Al-Pd-Mn,

Zn-Mg-RE and Al-Ni-Co alloys [4-10]. Concerning the point of departure, one has to state that it was rather disadvantageous. What concerns phase radiographic investigations (a method that has rather low sensitivity to the structural quality) of the mentioned three systems, we disposed of rather numerous experimental material. This was contrary to the situation of the X-ray topographical results. Only the icosahedral Al-Pd-Mn phase is well investigated by this highly sensitive method, and notabene, this was done mainly at the ESRF, due to its unique and well-adopted station ID19. Nearly no results exist for the decagonal Al-Ni-Co alloys - neither in the own lab, nor in the published literature. So we were obliged to look over a rather large amount of new and not so new samples to find those of acceptable crystalline quality and to create in this way an appropriate experimental basis for the future work. Consequently the work had to be concentrated on X-ray topographic investigations.

Figures 1 and 2 show X-ray topographs in diffraction geometry of the new icosahedral CdYb and ZnMgSc alloys. The CdYb single grains were grown by Bridgman technique in the Ames Laboratory. The i-ZnMgSc icosahedral phase was grown by slow cooling from the melt and then quenched in water [3]. Due to the facts that these alloys consist on rather absorbing elements and that we only disposed of bulky as grown samples (no thinned plates), we had to work in reflection geometry. The images show orientation contrasts of several grains. No individual defect contrasts are visible. The high defect density appears as rather homogeneous (averaged) contrast of the individual grains. This is supported by the fact that the measures global misorientation of the grains is about 0.25º. This is one order of magnitude larger than the average value for good quality Al-Pd-Mn samples (compare fig. 4). The same holds for the investigated dodecagonal AlCoNi samples. One of the best of them is presented in fig. 3. This one of the first and best topographs ever obtained from a dodecagonal quasicrystal. For conparison fig. 4 shows an example of an X-ray topograph of a “high quality” Al-Pd-Mn sample, having a measured global misorientation of the grains of about 0.25º, but local misorientations in spots of the order of $50*50\mu m^2$ within one grain (compare report HS-2088) of about 0.001degrees! As a consequence of those investigations we have to state that much more beamtime for detailed studies is necessary to reach the above-mentioned goal.

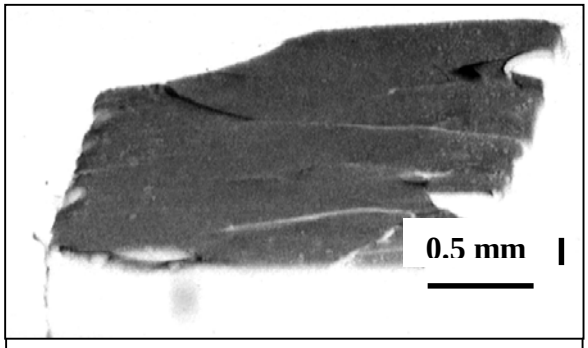

Fig. 1: X-ray topograph of i-CdYb in reflection geometry. Diffraction vector perpendicular to crystal surface, τ^3(0/2 0/0 0/0)-reflection, 2-fold axis, integrated over rocking angle 0.29°, sample-to-film distance $d_{s\text{-}f}$ = 4.5 cm, beam energy 24keV. Vertical image direction contracted by a factor 0.26.
Orientation contrasts of several grains are visible.

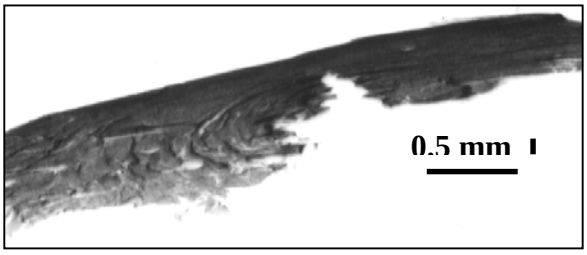

Fig. 2: X-ray topograph of i-ZnMgSc in reflection geometry. Diffraction vector perpendicular to crystal surface, τ^7(0/2 0/0 0/0)-reflection, 2-fold axis, integrated over rocking angle 0.25°, sample-to-film distance $d_{s\text{-}f}$ = 7.5 cm, beam energy 24keV. Vertical image direction contracted by a factor 0.17.
Orientation contrasts of several grains are visible.

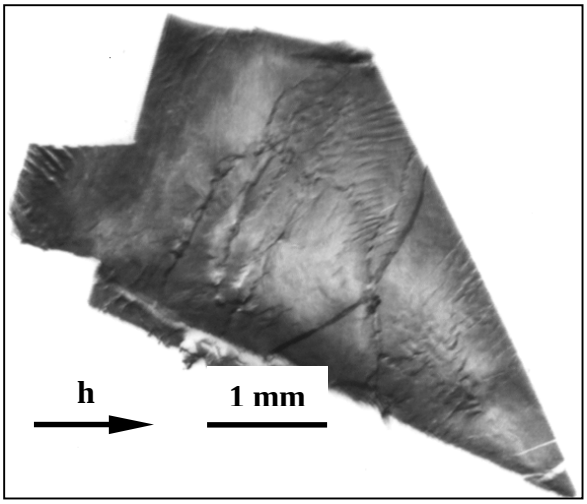

Fig. 3: X-ray topograph of dodecagonal AlCoNi in transmission geometry. **h** - diffraction vector, (1 0 0 –1 0)-reflection, integrated over rocking angle 0.25°, sample-to-film distance $d_{s\text{-}f}$ = 7.5 cm, beam energy 24keV.
Orientation contrasts of several grains are visible.

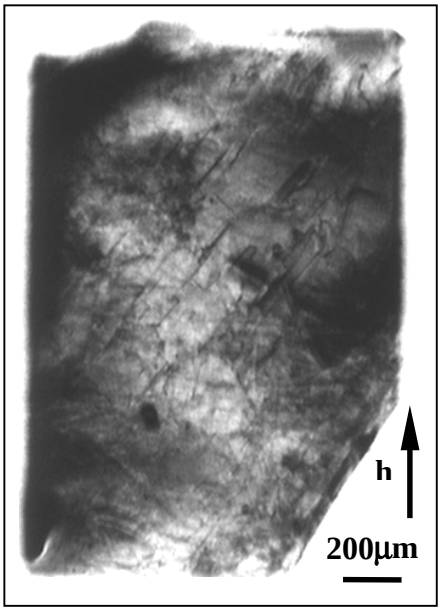

Fig. 4: X-ray topograph of i-AlPdMn in transmission geometry. Reflection τ^3(0/2 0/0 0/0), 2-fold axis, rocking angle 0.025°, sample-to-film distance $d_{s\text{-}f}$ = 4cm, beam energy 24keV. **h** - diffraction vector.
Contrasts due to global bending, dislocations, pores and two-dimensional defects are visible.

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