ESRF	**Experiment title:** **Atomic structure of the CdYb icosahedral phase**	**Experiment number**: HS1559
Beamline:	**Date of experiment**: from: 23 01 2002 to: 05 02 2002	**Date of report**: 29 07 2002
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Report:

In recent years a lot of effort has been dedicated to the understanding of the atomic structure and physical properties of quasicrystals. For icosahedral phases, which are 3 dim quasicrystals, most of the studies have been focussed on two systems where it is possible to obtain large single grains of the icosahedral phase with a very good structural quality: i-$Al_{70}Pd_{20}Mn_{10}$ (1) and i-Zn_6Mg_3Y (2). The most effective approach for structural determination of quasicristals is the 6-dim crystallography where periodicity is recovered in a high dimensional space. Although large progress have been achieved and realistic atomic models have been proposed, the agreement with the observed data is far from what is achieved in standard crystallography: whereas the strongest reflections are well reproduced, the weakest one fail to be properly reproduced (3). In short, only a first order approximation has been proposed and the problem of the structure of quasicrystals remains a challenging one. In particular it has not been yet possible to give an answer on the existence of chemically defined atomic clusters, on the importance of chemical disorder, all points which are crucial for the understanding of the growth and of physical properties of quasicrystals.

The recent discovery of a stable icosahedral $Cd_{85}Yb_{15}$ phase by the group of A.P. Tsai (4) is a breakthrough in the quasicrystalline field for several reasons: (i) it is the first quasicrystal in the Cd system; (ii) it is the first stable *binary* quasicrystal (all other stable QC are ternary phases); (iii) it is the first stable icosahedral phase with a Pm35 space group (other stable i-phases have a Im35 space group; (iv) there is a cristalline approximant phase with almost the same composition (Cd6Yb, Im3 space group, a=1.56 nm) whose structure is known. The elementary atomic clusters which are found in this periodic structure are completely new, with an inner part which has no icosahedral symmetry.

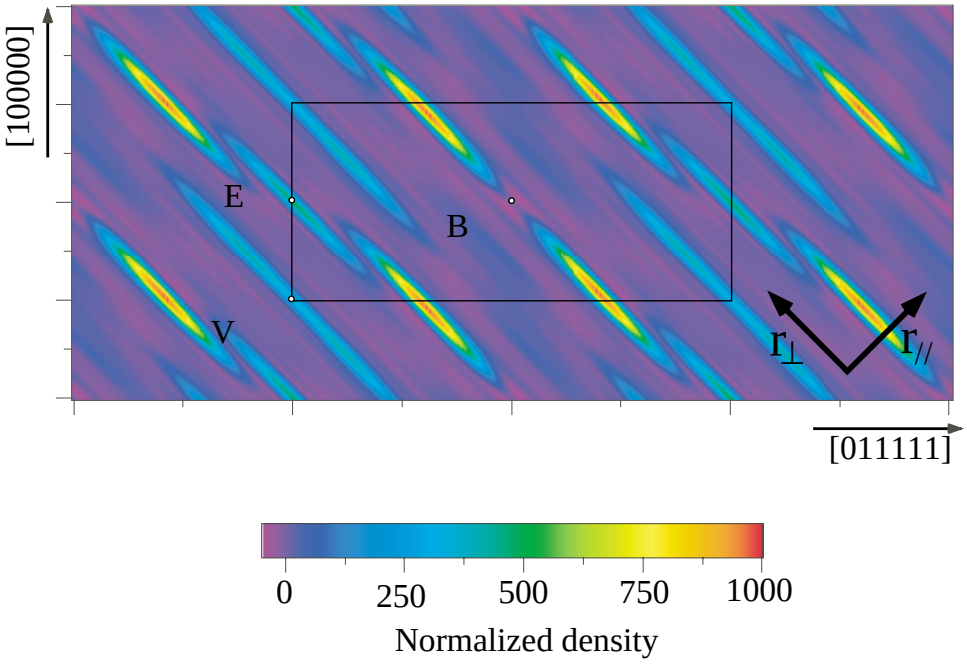
Experimental details: A single grain of the i-CdYb phase, with a cubic size of approximately 0.3 mm, was extracted from an ingot slowly cooled from the liquid. It was sealed under inert gas in a glass capillary to avoid oxydation. The incoming X-ray energy was set to 20.6 keV, to minimise absorption corrections. The

sample quality has been checked carefully, in particular with respect to phason disorder. We found a sharp sample mosaic (0.03° FWHM) and a Bragg peak broadening which scales with Qper. The broadening is similar to what had been found in the ZnMgY phase. There is also a visible amount of diffuse scattering around the Bragg peaks, due to long wavelength phason fluctuations.

For data collection we used the continuous fast scan procedure. Once the orientation matrix was refined, the proper filter was automatically selected, and the scan carried out. This procedure allows the measurement of about 1000 reflections in 24 h. The scanning width was adapted according to the Qper value of the diffraction vector, which was varying between 0 and 3 (unit less value). In order to check for possible beam instability, a standard reflection has been measured regularly. Its variation was found to be very small and smooth as a function of time, with maximum amplitude variation of 20% during 7 days of measurement. A few reflections were measured in an other asymmetric unit, and all accessible equivalent reflections were measured for 10 reflections.

Data have been integrated and corrected for absorption. Equivalent reflections and re-measured one were found to agree within 4%. Altogether 5500 independent reflections have been integrated, with a dynamical range larger than 7 orders of magnitude in the intensity

Data analysis: A subset of 1000 reflections has been used for phase reconstruction, using the low density elimination method [5]. By FT of this data set, 6D density map have been recorded. The figure shows a section of the density map in a plane containing a 5-fold axis in physical (parallel) and complementary space (perp). There are three atomic surfaces located on the node (V), body-centre (B) and mide edge (E) of the 6D cube. The density is much larger on the B site, which indicate that it is mainly occupied by heavy Yb atoms (ZYb=70, ZCd=39).



The raw shape of the atomic surfaces could also be extracted. The B atomic surface presents an empty core. It is the same for the V atomic surface. From this starting point a 6D model has been constructed, and refined. This is in progress, but preliminary results give a 10% R-factor.

In conclusion a full data set has been collected in the CdYb phase. It is the first time that data with such a large dynamical range (7 orders of magnitude) could be measured in a quasicrystalline sample. The 6D structure is simple, with 3 different atomic surfaces. Although refining such a dataset is challenging, this should lead to detailed description of the i-CdYb atomic structure.

References

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