ESRF	**Experiment title:** Atomic structure of the ZnMgSc icosahedral phase.	**Experiment number**: **02 02 608**
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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.

The recent discovery of a stable icosahedral $Cd_{85}Yb_{15}$ phase by the group of A.P. Tsai (3) 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. From data collected at the ESRF a first model has been proposed for the i-CdYb phase, demonstrating that the same clusters as the one found in the approximant are present.

Recently the group of P. Ishimasa found a similar icosahedral phase in the ZnMgSc system (4): the Zn6Sc crystal, is isostructural with the Cd6Yb one. The icosahedral phase is obtained by a small Mg substitution, and has a composition $Zn_{81}Mg_4Sc_{15}$. When compared with the i-CdYb, this phase present less diffuse scattering.

Experimental details:

The experiment has been carried out on the D2AM beamline, using the 7-circle diffractometer. We worked at an energy of 9.3 keV, 0.36 keV bellow the Zn edge to avoid fluorescence. Integrated intensities were collected in the theta scan mode.

Single grains of the i- $Zn_{81}Mg_4Sc_{15}$ phase were prepared by slow cooling from the melt. A small spherically ground sample, with a diameter equal to 150μm, was extracted from the ingot. The strongest 350 reflections were collected with this sample. We then used a large single grain with a polished surface (3x3 mm2) oriented almost perpendicular to a 2-fold axis. With this sample we worked in reflection geometry, in a symetrical mode, so that absorption corrections are straightforward. In both cases a check reflection was measured regularly. After normalisation by the monitor, the standard deviation of the check reflection was found equal to 3% and 1% for the spherical and large sample respectivelly. With the large sample, weak reflections could be easily measured: 1550 reflections, with Qpar value between 0 and 8 and Qper values smaller than 3 have been collected. (Because of the time constraint only part of the reflections were collected for Qper between 2 and 3). A high dynamical range, with almost 7 orders of magnitude in intensity was achieved with this data set. Both data set (spherical and large sample) are consistent. In particular no extinction effect has been observed with the large sample: this is probably related to the relativelly high sample mosaic (about 0.05° with in general 2 blocks)

A first data analysis showed that the structure is similar to the one of the i-CdYb phase (5). The 6D analysis is illustrated by the density map shown on the figure which display a 5-fold section of the 6D structure. There are two atomic surfaces, located at the origin and on the mid edge. Similarly to what was obtained in the CdYb phase, the atomic surface located on the mid edge is made of 3 pieces, with a clear parallel component.

Further modeling using a cluster description is in progress, and should give information on the chemical order of the structure.

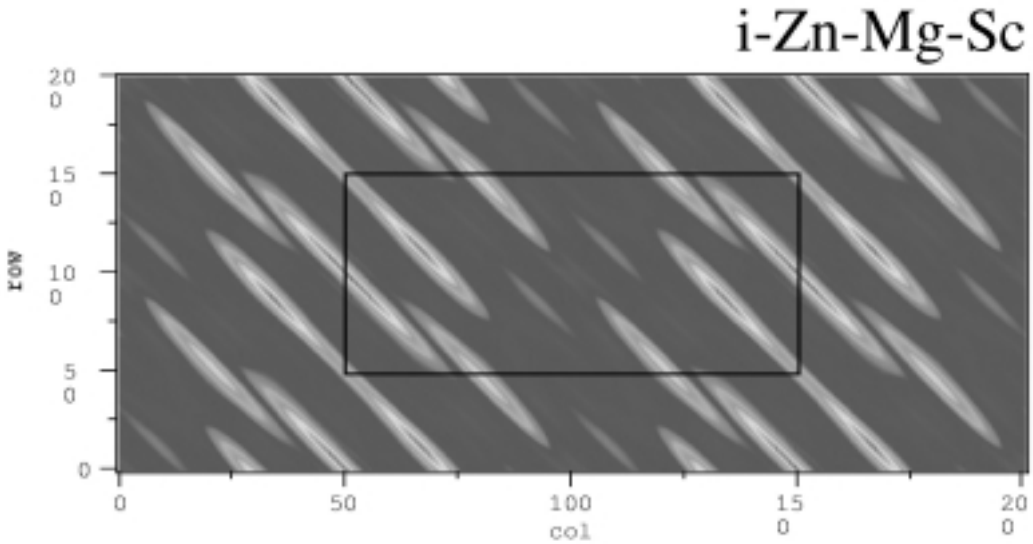

Figure: Typical electron density map obtained with the i-ZnMgSc phase. The figure is a section containing a 5-fold axis both in the physical and complementary perpendicular space. The trace of the unit cell is outlined.

References

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