ESRF	**Experiment title:** Local atomic structure in Cd-Mg-Tb quasicrystals by x-ray fluorescence holography	**Experiment number**: HC-4463
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Shifts: 15	**Local contact(s)**: Marc De boissieu (email: MArc.de-Boissieu@simap.grenoble-inp.fr) Nils Blanc (email: nils.blanc@esrf.fr) Gilbert Chahine (email: gilbert.chahine@esrf.fr)	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):
*Prof. Dr. Wolf-Christian Pilgrim, *Dr. Jens Stellhorn, *Benedict Paulus, *Jonathan Link Vasco (Philipps University Marburg, Germany), Dr. Marc De Boissieu (SIMaP, Grenoble), Prof. Dr. Shinya Hosokawa (Kumamoto University, Japan), Dr. Hiroyuki Takakura (Hokkaido University, Japan), Professor Koichi Hayashi (Nagoya Institute of Technology, Japan),

Report:

In this proposal, we planned to study the local atomic structure of a Cd-Mg-Tb icosahedral quasicrystal with X-ray fluorescence holography (XFH) with atomic-scale resolution. The aim was to elucidate the role of atomic disorder for the magnetic properties of the material.

As a method, XFH can directly visualize the local 3-dimensional (3D) atomic scale structure in physical space, without being impeded by the phase problem of traditional crystallography. This renders XFH unique as a tool to investigate the structure of quasicrystals.

We brought 2 sets of samples, i.e. quasicrystals and a two approximant crystals, for which the quality was confirmed beforehand. Unexpectedly however, we detected only a rather small signal (about 1 order of magnitude lower than expected from previous measurements), which was possibly related to the small sample and beam sizes and/or the low energy of the Tb Lα fluorescence. Therefore, it was necessary to change the sample system. We chose to continue our investigation of the decagonal Al-Co-Ni quasicrystalline system (Co and Ni holograms), for which we already measured initial data in a previous beamtime. Now, we were able to extend these measurements by higher energy holograms, which will provide an increased resolution for the real-space reconstructions and a improved reliability of the signals, which highly benefits the structural characterization of such complex (aperiodic) systems.

Decagonal quasicrystals such as the investigated Al-Co-Ni are described by a periodic stacking of quasiperiodic planes. Although their structure might seem simpler to tackle, there are still the subject of current studies because most of the decagonal phases display a significant amount of disorder, seen as diffuse scattering in the diffraction pattern and are ternary intermetallic

compounds [1, 2]. However, direct information on the local structure of quasicrystals is difficult – if not impossible – to obtain by conventional characterization methods. Here, XFH can support the structural determination because it is very sensitive to the positional fluctuations of neighbouring atoms, which can be estimated by comparing the image intensity and theoretical calculations [3].

The XFH measurements have been carried out on a large single grain sample, above the Ni and Co edge so that the average 3D local environment could be reconstructed around those two elements. We recorded 8 holograms with incident energies between 12.5 keV and 16.5 keV, which can be added to our previously recorded data between 8.5 and 12.0 keV. An exemplary hologram at 15.25 keV is shown in Fig. 1 and compared with a hologram obtained from computer simulation of a model structure [4,5], indicating a good agreement. The reconstruction of the real space information in the plane containing the emitter atom is shown in Fig. 1 c).

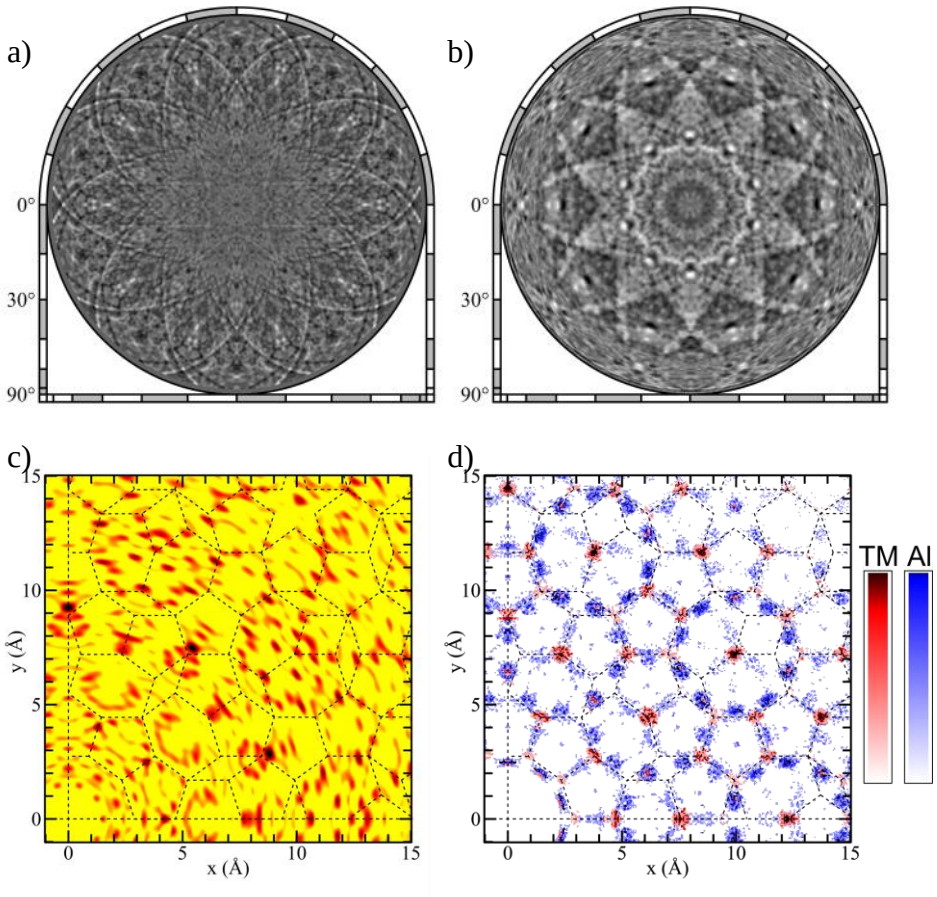

Fig. 1: AlCoNi data. (a) hologram at 15.25 keV in comparison with a hologram obtained by computer simulation (b), and reconstruction from the exp. data (c) in comparison with a projection of the average structure around Co (d).

References

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