ESRF	**Experiment title:** Local atomic structures in precipitation strengthening Al-Cu-Li alloys by X-ray fluorescence holography	**Experiment number**: 02-02-852
Beamline: BM02	**Date of experiment**: from: 21.09.2017 to: 26.09.2017	**Date of report**: 10.09.2020
Shifts: 15	**Local contact(s)**: Marc De Boissieu, Nathalie Boudet, Nils Blanc	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Jens R. Stellhorn*1, S. Hosokawa*1, B. Klee*1, K. Hayashi*2, Artoni Ang*2, M. de Boissieu*3,

1 Philipps-Universität Marburg, Fachbereich Chemie, Hans Meerwein Strasse, Marburg 35032, Germany
2 Structural Physics Laboratory, Nagoya Institute of Technology, Japan
3 Science et Ingienerie des matériaux et procédés, St. Martin d'Heres, CEDEX

Report:

X-ray fluorescence holography (XFH) is a relatively newly developed technique of structural characterization. It is element-specific and provides information on the atomic scale local environment. By using the XFH technique, we planned to investigate the local structure around Cu atoms in Al-Cu-Li based alloys for the first time. The results were expected to give detailed information on the role of Cu in the precipitates and the correlation between Cu and Al atoms, which is a crucial information to produce improved light-weighted alloys. Unexpectedly, it was found that the Al-Cu-Li single crystal actually contained 2-3 grains in different orientations, which made the characterization with XFH impossible, which requires a pure single-crystal sample since it determines the average structure as a superposition of all atoms of the same elements in the structure.

Therefore, it was necessary to exchange the sample. We were able to investigate a different, though fairly complex, system: a quasi-crystal of Al72Co9Ni19. Quasicrystals are long range ordered structures that lack translational invariance [1]. Their diffraction pattern displays sharp Bragg peaks but with symmetries incompatible with lattice translation [2]. Their structure is usually best understood using the superspace crystallography approach developed for aperiodic crystals [1]. Decagonal quasicrystals 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 [3, 4].

However, direct information on the local structure of quasicrystals is difficult – if not impossible – to obtain by conventional characterization methods. Therefore, we applied the x-ray fluorescence holography (XFH) technique to explore the atomic configurations in this decagonal quasicrystal. In particular, XFH can support the structural determination of this material because it is very sensitive to the positional fluctuations of neighboring atoms, which can be estimated by comparing the image intensity and theoretical calculations [5].

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 8.5 keV and 12.0 keV. The data were corrected for the fluorescence background and expanded using the 10-fold symmetry of the quasicrystal lattice. From these holograms, we reconstructed the [00001] plane around the Co and Ni atoms, the latter is shown in Fig. 1 (a). The structure is compared with a model obtained from a first principles calculation [7], for which the corresponding holograms were simulated and the real-space again reconstructed (b), as well as with the direct projection of the average structure from the model (c). The basic motifs of the quasicrystal according to the average lattice (indicated by the lines) are well represented, but several artificial features still exist owing to the complex structure of the material. Additional holograms measured at a higher energy would be able to solve the deviations from the expected structure.

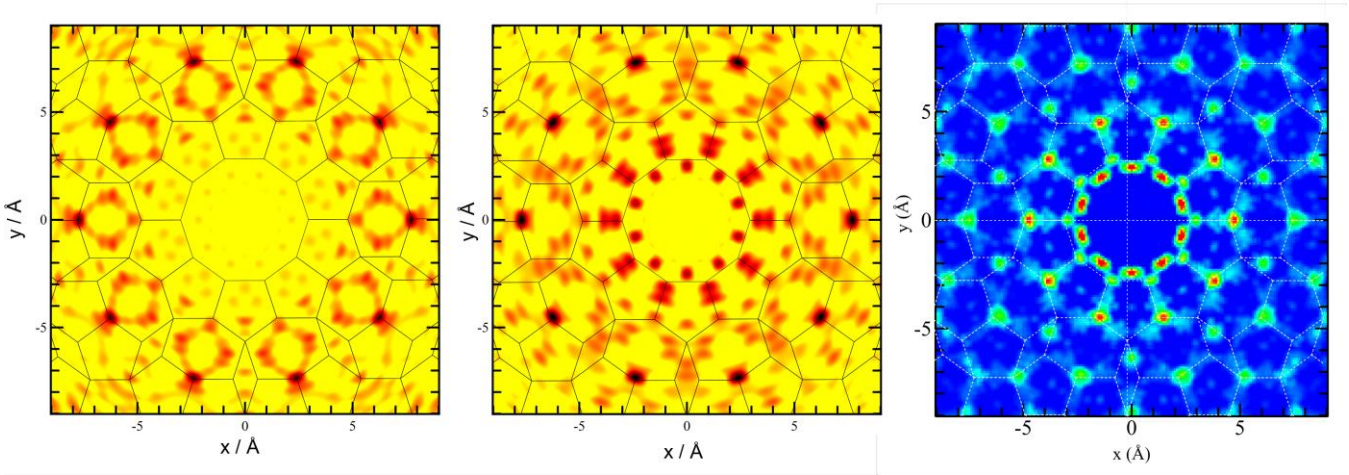

Fig. 1: AlCoNi structure. (a) reconstructions from exp data and (b) from a computer simulation. (c) projection of the average structure around Ni after [7].

References

[1] T. Janssen, G. Chapuis and M. de Boissieu, Aperiodic Crystals. From modulated phases to quasicrystals, Oxford University Press, Oxford, 2007.
[2] D. Shechtman, I. Blech, D. Gratias, et al. Phys. Rev. Lett. 53, 1951 (1984).
[3] W. Steurer, S. Deloudi, Crystallography of quasicrystals, Springer, 2009.
[4] W. Steurer, Z. Kristallogr. 219, 391 (2004).
[5] K. Hayashi et al., J. Phys.: Condens. Matter 24, 093201 (2012).
[6] C.L. Henley, J. Alloys and Compounds 342, 221 (2002).
[7] M. Mihalkovic, M. Widom and C.L. Henley, Phil. Mag. 91, 2557-66 (2010).