Atomic resolution holography for characterizing the local structure in quasicrystals

Jens R. Stellhorn[1], Shinya Hosokawa[2], Koji Kimura[3], Kouichi Hayashi[3], Natalie Boudet[4], Nils Blanc[4], Gilbert Chahine[4], Marc de Boissieu[5]

[1]Dept. of Applied Chemistry, Hiroshima University, Higashi-Hiroshima 739-8527, Japan,

[2]Dept. of Physics, Kumamoto University, Kumamoto 860-8555, Japan,

[3] Dept. of Physical Science and Engineering, Nagoya Institute of Technology, Aichi 466-8555, Japan,

[4]Univ. Grenoble Alpes, CNRS, Institut Néel, Grenoble 38042, France,

[5]Univ. Grenoble Alpes, CNRS, SIMaP, Grenoble F-38000, France

stellhoj@hiroshima-u.ac.jp

The atomic-resolution holography (ARH) technique [1,2] offers the possibility to experimentally determine the local atomic-scale structure of quasicrystals. This method can selectively investigate specific elements and their 3-dimensional local atomic environment in a range of up to around 2 nm, without the need of *a priori* information on the structure. Therefore, it can provide a novel perspective for the visualization of the structure of aperiodic systems.

Recently, we have described the results of the ARH reconstruction for the Penrose lattice, which can be regarded as a reference system for decagonal quasicrystals. The resulting pattern of atomic images can be interpreted a projection of the average structure.[3] Using this framework, we can now describe how the experimental results for decagonal Al-Co-Ni quasicrystals compare with the projection of the average structure from a computational model.[4]

An example is shown in the Figure below, with exemplary data of an experimental hologram of an Al-Co-Ni quasicrystal (a). The intense lines in the hologram are the so-called X-ray standing wave lines, which indicate the 10-fold symmetry of the system. The reconstruction of the environment around the Co atoms from the holograms is illustrated in (b), and is compared with the corresponding projection from the computational model (c). Shown here is the quasi-periodic plane that includes the emitter atom at the origin. The atomic images at the vertices of the dashed polygons can be identified with transition metal atoms, while Al atoms are mainly distributed along the polygon edges.

We will also demonstrate the differences of the quasiperiodic structure versus a crystalline approximant and illustrate the ARH results for icosahedral structures.

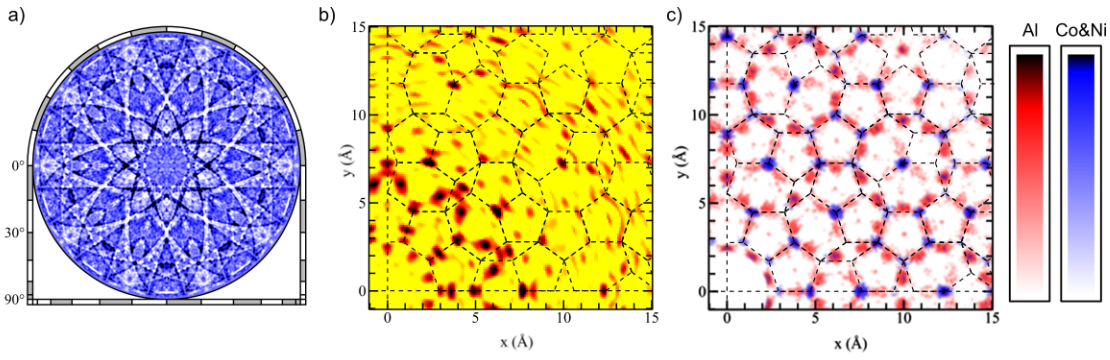

Figure 1. (a) X-ray Co K_α hologram of decagonal Al-Co-Ni sample measured at 10 keV, measured at BM02 / ESRF. (b) Reconstruction of the average structure around the Co atoms from the experimental holograms, and (c) the projection of the average structure from a computational model [4]. The dashed lines indicate the average structure of the Penrose tiling [3].

[1] M. Tegze and G. Feigel (1996), Nature **380**, 49.

[2] K. Hayashi et al. (2012), J. Phys.: Condens. Matter **24**, 093201.

[3] J. R. Stellhorn et al. (2021), Mater. Trans. **62**, 342-349.

[4] M. Mihalkovic et al. (2010), Phil. Mag. **91**, 2557.

Keywords: quasicrystal; atomic resolution holography; local structure; site selectivity