MS23 Quasicrystals and complex intermetallic materials

MS23-04
Atomic Resolution Holography to Study the Local Structure in Quasicrystals
J.R. Stellhorn [1], K. Kimura [2], K. Hayashi [2], N. Happo [3], N. Fujita [4], S. Ohhashi [4], M. De Boissieu [5]

[1]Hiroshima University - Higashi-Hiroshima (Japan), [2]Nagoya Institute of Technology - Nagoya (Japan), [3]Hiroshima City University - Hiroshima (Japan), [4]Tohoku University - Sendai (Japan), [5]University Grenoble Alpes - Saint-Martin-d'Hères (France)

Abstract
The atomic-resolution holography (ARH) technique [1-3] offers the possibility to experimentally determine the local atomic-scale structure of complex systems. 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, like quasicrystals. Owing to the high complexity of the atomic arrangements in these systems, techniques targeted at the local atomic structure can provide valuable complementary information to understand the crystal chemistry (in addition to e.g. superspace crystallography approaches).

The local perspective of the structure by ARH provides an average view around a specific element in 3-dimensional space. In this presentation, we will show the recent developments for the ARH structure determination for decagonal and for Tsai-type icosahedral systems, in particular the evolution from approximant to quasicrystalline systems. Due to the 3D information available from ARH, we can for example distinguish between intra- and inter-cluster correlations of the icosahedral clusters. Some results from the investigation of a 2/1 approximant (AP) of the Ag-In-Yb system are illustrated in the figures below.

Fig.1: (a) The spherical hologram of a AgInYb 2/1 AP measured at 9.5 keV.
(b, c) 3D reconstructions of the ARH data, highlighting the atomic images related to the connections inside (blue) and between (purple) the Yb icosahedra, both having interatomic distances of about 5.7 Å.
(d) Structural view in real space along the pseudo-5-fold axis of the approximant.

References
[1] M. Tegze, G. Feigel, Nature 380 (1996) 49
[2] K. Hayashi et al., J. Phys.: Condens. Matter 24 (2012) 093201
[3] J. R. Stellhorn et al., Mater. Trans. 62, (2021) 342-349

Figure 1