Investigating the local structure of icosahedral phases by Atomic Resolution Holography


1 Nagoya University, Nagoya, Japan, 2 Hiroshima University, Hiroshima, Japan, 3 Nagoya Institute of Technology, Nagoya, Japan, 4 Hiroshima City University, Hiroshima, Japan, 5 Tohoku University, Sendai, Japan, 6 University Grenoble Alpes, Saint-Martin-d’Hères, France

jens.stellhorn@nagoya-u.jp

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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, 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, it is possible for example to 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 figure below. The ARH data can also support the understanding of the relationship between magnetic properties and the aperiodic structure, which we investigated for the Cd-Mg-RE system (RE = rare earth). Here, the magnetic characteristics were recently investigated and attributed to the positional (and chemical) disorder of Cd and Mg sites.[4,5] The direct observation of the underlying atomic arrangements is difficult by conventional methods, and the ARH measurements offer a unique new insight into this phenomenon.

Figure 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.