Unravelling complex systems through diffuse scattering

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Increasingly, materials with structural and/or dynamical disorder are studied with crystallographic methods, which were considered for many years only able to show perfectly periodic arrangements. In reality, this perfect periodicity simply describes an average reconstruction of the structure, and the disorder adds a supplementary signal, found as diffuse scattering. Its analysis can be helped with a look to the real space, using the Pair Distribution Function, modelling the disorder with Monte Carlo methods and so on. This talk will explore different cases giving an emphasis on the design of the materials, the use of advanced total scattering techniques and the link to functional properties.

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Investigation of the Local Atomic Structure of Quasicrystals by Atomic Resolution Holography

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Atomic-resolution holography (ARH) enables the determination of the local atomic-scale structure of complex systems in a wide range [1-3]. This method selectively investigates specific elements and their 3-dimensional local atomic environment, without the need of *a priori* information on the structure. This provides a unique perspective in particular for the visualization of the structure of aperiodic systems. Because of their high complexity on the atomic scale, techniques targeted at the local atomic structure can offer valuable complementary information to understand the aperiodic crystal chemistry.

In this presentation, we will show the recent developments for the ARH structure determination for aperiodic systems, in particular the evolution from approximant to quasicrystalline structures. The 3D information available from ARH makes it possible e.g. to visualize correlations between the Tsai-type clusters in icosahedral materials: as illustrated in the Figure below, we can distinguish between intra- and inter-cluster correlations of the icosahedral Yb-clusters in the Ag-In-Yb system. Both correlations appear at similar lengths (about 5.7 Å) but with different spatial arrangements in 3D. Our investigation also focuses on the relationship between the aperiodic structure and material properties, for example the magnetic properties of the Cd-Mg-RE system (RE = rare earth), which were recently attributed to the positional (and chemical) disorder of Cd and Mg sites [4,5]. Since the direct observation of the underlying atomic arrangements is difficult using conventional methods, the ARH measurements offer a new insight into the phenomena on the atomic level.

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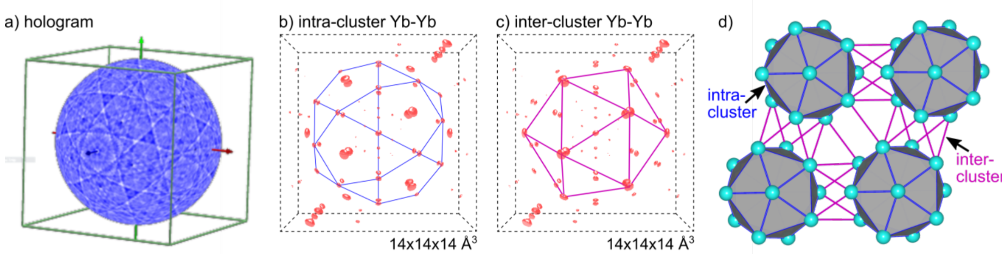

Fig. 1: (a) The spherical hologram of a AgInYb 2/1 AP measured at 9.5 keV. (b, c) 3D reconstructions of the ARH data, highlighting the atomic images related to the connections inside (blue) and between (purple) the Yb icosahedra, both having inter-atomic distances of about 5.7 Å. (d) Structural view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