	Experiment title: Atomic configurations and positional fluctuations in decagonal phase Al ₇₅ Ni ₁₀ Co ₁₅ quasicrystal by x-ray fluorescence holography	Experiment number: HC-3434
Beamline: BM02	Date of experiment: from: 8 Nov 2017 to: 14 Nov 2017	Date of report: 02 / 02 / 2018
Shifts: 18	Local contact(s): Nathalie Boudet, Nils Blanc, Marc de Boissieu	<i>Received at ESRF:</i>
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Report:

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 an Al₇₃Ni₁₂Co₁₅ decagonal quasicrystal. XFH is a newly developed technique for structural characterizations [5]. By irradiating x-rays with an energy higher than an absorption edge of a constituent element, an interference of the incident x-rays occurs between the direct ones (reference wave) and those scattered by the surrounding atoms (object wave). As a result, a modulation in the fluorescent x-ray intensity from the emitter atom is generated by about some $\pm 0.1\%$, and its crystal angle dependence is obtained, which is called a hologram. By calculating a simple Fourier transform of the hologram, three-dimensional (3D) atomic images can be reconstructed around a specific element emitting the fluorescent x-rays. Moreover, we found that XFH 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. One of the obtained holograms is shown exemplarily in Fig. 1. X-ray standing wavelines are clearly observed and indicate the quasi-crystallinity of the sample. From these holograms, we reconstructed the xy plane around the Co and Ni atoms, the latter is shown in Fig. 2. These images can be used to analyze the local structure in detail, and allow us to compare the results with well-known structural features, e.g. the "20 Å clusters", which are observed as a decagon with a diameter of about 20 Å and with Al atoms on the vertexes, corresponding to the outermost signals in Fig. 2. Additionally, we observe two other decagons (dashed lines in Fig. 2), which are well in agreement with theoretical predictions (e.g. [6, 7]). The intensity ratio correspond to the expected decoration of the vertex positions, i.e. Al (small intensity) on the inner and outer decagon, and Ni and Co atoms on the vertexes of the medium decagon (higher intensity). Further analysis of the structure is now in progress.

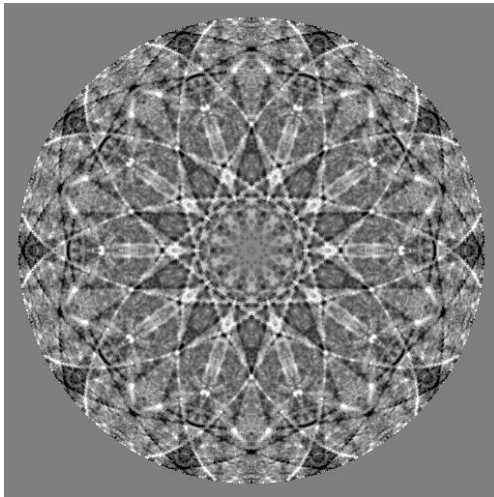


Fig. 1: Orthogonal projection of the Co K-alpha hologram measured at 10.5 keV incident energy. The hologram is centered at $\theta=0^\circ$ and the radial and angular direction indicate θ and ϕ , respectively.

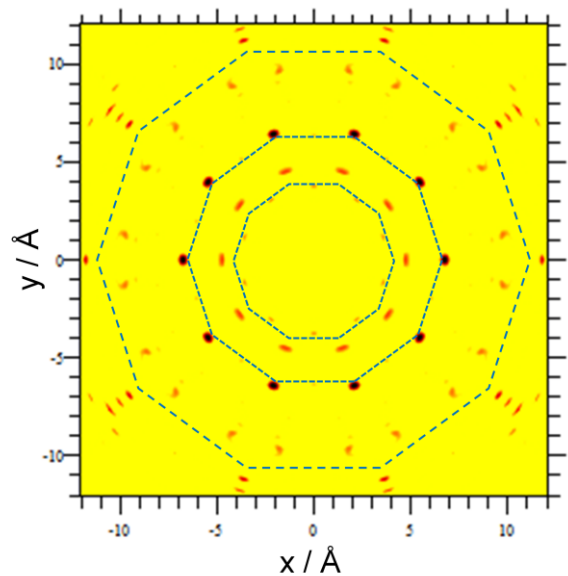


Fig. 2: Atomic image reconstruction of the xy plane around a Ni atom, from 8 holograms. Dashed lines indicate predictions of decagonal features from computer simulations [7].

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