ESRF	**Experiment title:** Structure determination of decagonal $Al_{70.5}Mn_{16.5}Pd_{13}$ quasicrystal	**Experiment number:** HC-357
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Report:

The decagonal phase $Al_{70.5}Mn_{16.5}Pd_{13}$ belongs to the class of decagonal quasicrystal with ~12 Å translational periodicity [1]. The diffraction pattern exhibits a large set of sharp Bragg peaks besides strong diffuse scattering. Based on a data set collected with an in-house diffractometer a first crude structure model (wR = 0.214) could be derived [1] in the decagonal space group $P10_5/mmc$ (d_1,...,d_4 = 3.482(5) Å; d_5 = 12.585(2) Å α_{ij} = 60°, α_{i5} = 90°, i,j = 1,...,4; V = 1039(6) Å^5). However, the structure solution was severely biased by the big amount of structured diffuse scattering phenomena (Fig. 1).

To characterize the sample quality high-resolution two-dimensional scans of 23 selected peaks were performed. The sample shows peak splitting (Fig. 2). Several states of ordering like quasicrystal, nanodomain structure or multiple twinned approximants have to be considered. As observed in decagonal A1-Co-Ni alloys [2] there exists peak splitting which cannot be described by simple twinning as peak positions do not agree with the predicted ones. However, simulations assuming coherent ordering of nanodomains [3] are in good agreement with the observed data. The same argumentation could now be applied to the decagonal A1-Mn-Pd phase. The large amount of high resolution data allows different models to be distinguished.

Based on the analysis of the two-dimensional peak profiles (mosaic spread of 0.08°) a data collection using a wavelength of 1.000 Å (μ = 186 cm-') was performed and resulted in 3781 reflections. To obtain a homogeneous data set (sin $\theta/\lambda < 1.2$ Å^{-1}) with high resolution also in the perpendicular space all reflections within two asymmetric units in the five-dimensional description were selected. Merging of all reflections resulted in 1868 unique reflections. A detailed peak profile analysis allows diffuse scattering phenomena to be separated from Bragg peaks. The remaining reflections with high perpendicular component of their scattering vector will be used for an detailed analysis of the acceptance domains of the corresponding hyperatoms.

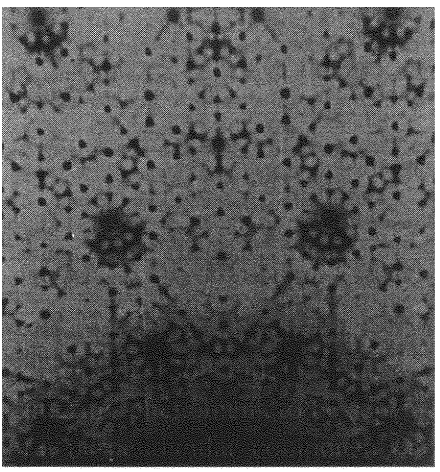

Fig. 1: Precession photograph of the 0th layer of decagonal $Al_{70.5}Mn_{16.5}Pd_{13}$.

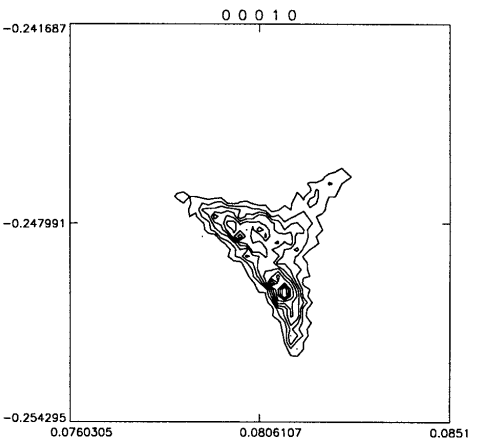

Fig. 2: High-resolution scan of the 00010 reflection. Units: Å^{-1}.

[1] Steurer, W., Haibach, T., Zhang, B., Beeli, C., Nissen, H.-U.: *The Structure of Decagonal* $Al_{70.5}Mn_{16.5}Pd_{13}$. J. Phys. Condens. Matter 6 (1994) 613-632.

[2] Kalning, M., Press, W., Kek, S.: *Investigation of Decagonal* $Al_{70}Co_{15}Ni_{15}$ *Single Crystals by Means of High-resolution Syncrotron X-ray Diffraction.* Phil. Msg. Lett. 71(6) (1995) 341-349.

[3] Steurer, W., Honal, M., Haibach, T.: *Mechanism of the Phase Transformation in Decagonal Phases.* Proceedings of 5th International Conference on Quasicrystal ICQ95. Singapore - World Scientific, in press.