

**Experiment title:**Structure determination of decagonal
 $A_{1.71}Fe_5Ni_{2.4}$ quasicrystal**Experiment****number:**

HC-589

Beamline:

D1-SW/NO

Date of experiment:

from: 30/01/96

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Date of report:

06/02/96

Shifts:

15

Local contact(s):

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The novel [1] decagonal quasicrystalline material $A_{1.71}Fe_5Ni_{2.4}$ shows almost none of the predominant diffuse scattering phenomena (Fig. 1), typical for decagonal phases [2].

To characterize the sample quality two-dimensional scans of selected Bragg peaks, which are most sensitive on twinning, have been performed (Fig. 2). No peak splitting according to multiple twinned approximants or nanodomain structures could be observed. The high-resolution scans only show a peak broadening due to mosaicity. The FWHM using a wavelength of 0.55 Å is 0.0129°, indicating a ‘good’ quality decagonal quasicrystal. The quasiperiodic metrics could be verified with high accuracy ($d_1, \dots, d_4 = 3.7295(6)$ Å, $d_5 = 4.0969(5)$ Å, $\alpha_{ij} = 60^\circ > \alpha_{i5} = 90^\circ > i, j = 1, \dots, 4$).

The data collection was performed using a wavelength of 0.55 Å ($\mu = 48.4$ cm⁻¹) and resulted in 9240 reflections. To achieve a homogeneous data set with high resolution in the five-dimensional description, all reflections within two asymmetric units ($\sin \theta_\lambda \leq 2.0$ Å⁻¹) have been measured. Merging of these reflections resulted in 4331 unique reflections.

As the extinction rule

$$h_1 h_2 \bar{h}_2 \bar{h}_1 h_5, h_5 = 2n + 1$$

is strictly obeyed, the five-dimensional space group $P10_3/mmc$ will be used in the first data analysis.

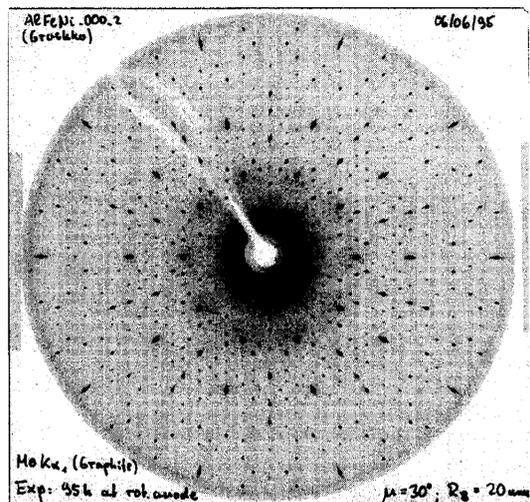


Fig. 1: Precession photograph of the 0th layer of decagonal $Al_{71}Fe_5Ni_{24}$.

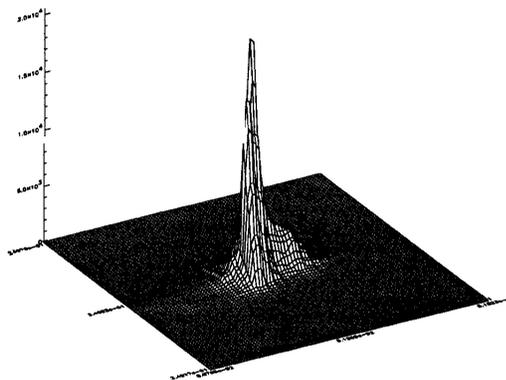


Fig. 2: High resolution scan of the 10000 reflection. Area: $1.1 \cdot 10^{-3} \text{ \AA}^{-1} \times 1.5 \cdot 10^{-3} \text{ \AA}^{-1}$.

- [1] Lemmerz, U., Grushko, B., Freiburg, C., Jansen, M.: *Study of Decagonal Quasi-crystalline Phase Formation in Al-Fe-Ni alloy system*. Phil. Msg. Lett. 69 (1994) 141-164.
- [2] Steurer, W., Haibach, T., Zhang, B., Kek, S., Luck, R.: *The Structure of $Al_{70}Ni_{15}Co_{15}$* . Acts Crystallogr. B49 (1993) 661-675.
- [3] Haibach, T., Estermann, M. A., Steurer, W., Kalning, M., Kek, S.: *High Resolution Measurement of Decagonal $Al_{70}Co_{15}Ni_{15}$ Optimised for Atomic Surface Determination*. Conference Proceedings of ICQ95. Singapore - World Scientific (1995) in press.