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ESRF

# Experiment Report Form

**The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF**.

Once completed, the report should be submitted electronically to the User Office via the User Portal:

*https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do*

***Reports supporting requests for additional beam time***

Reports can be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

***Reports on experiments relating to long term projects***

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

***Published papers***

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

## Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

## Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

| ESRF | **Experiment title: X-ray structure analysis of the new two-dimensional dodecagonal oxidic quasicrystal** | **Experiment number**: HC-1437 |
|---|---|---|
| **Beamline**: | **Date of experiment**: from: Sep. 20, 2014 to: Sep. 30, 2014 | **Date of report**: Jul. 19, 2015 |
| **Shifts:** | **Local contact(s)**: R. Felici | *Received at ESRF:* |

**Names and affiliations of applicants** (* indicates experimentalists):

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**(3) Katayoon Mohseni (*); as (1)**

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**(5) R. Hammer (*); as (2)**

**(5) Wolf Widdra (*); as (2)**

**(6) J. Kirschner; as (1)**

**Report:**

**It was the aim of the study to investigate the atomic structure of the recently discovered dodecagonal oxidic quasicrystal (QC) [1] using surface x-ray diffraction. The experiments could be carried out very successfully. Reflections of the QC and its periodic approximant (PA) were collected. The data analysis has been carried out using standard methods of crystallography. Here, we shortly report on the results obtained for the PA.**

**Fig. 1 shows the STM images of the QC (a) and the PA (b), both prepared on Pt(111), as well as the corresponding LEED pattern (c) [1]. The QC reflections are very weak and indicated, those of the PA appear as sharp and well contrasted spots. The STM images are very similar showing bright spots which are arranged in the Stampfli-Gähler- [2,3] and the Kepler tiling [4] in the case of the QC and the PA, respectively.**

**Fig. 2 shows the Fourier-synthesis of the z-projected charge density [ρ(x,y)] of the PA calculated on the basis of 44 symmetry independent structure factors of type $F_{hk0}$ (plane group symmetry p2). In total, four unit cells are displayed. The charge density plot shows a number of strong and weak peaks. It also allows to identify the Kepler-tiling visible in the STM image and which -according to the SXRD anaylsis- now can be unambiguously related to titanium atoms.**

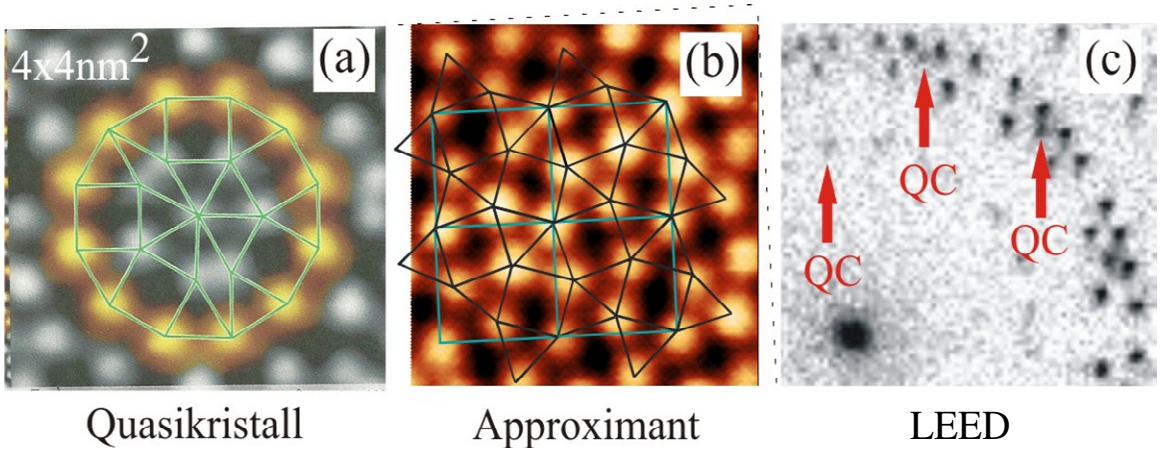
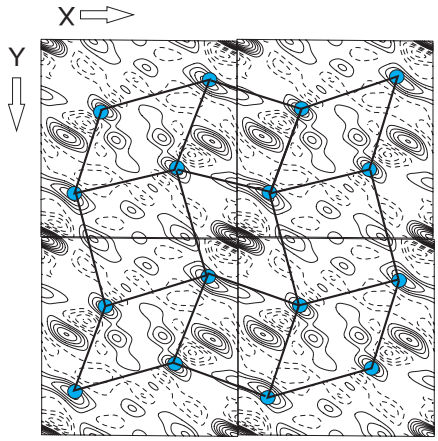



**Fig.1: STM images of the QC (a) the PA (b) and the LEED pattern (c) (from Ref. [1]). Bright spots in STM are related to titanium atoms according ot the SXRD analysis.**




**ρ(x,y) of approximant**

**Fig.2: Z-projected Charge density of the PA phase shown for four unit cells. Peaks which correspond to the Kepler tiling are highlighted for comparison with the STM image. Note that there is a shift of the origin of the unit cell in Fig.2 relative to Fig.1 (b) in accordance with the p2 symmetry.**

**Other strong and weak peaks correspond to barium and oxygen atoms, respectively. The fit of the calculated $|F|^2$ values to the experimental ones on the basis of this structure model yields an unweighted R-value of 14% based on $|F|^2$.**
**In summary, we have carried out a SXRD analysis of the two-dimensional oxidic PA and the QC structure. In combination with state-of-the-art first-principles calculations our results also allow a deeper insight into the principles which govern their stability and which lead to their formation. More details will be discussed elsewhere [5].**

**This work is supported by the DFG through SFB 762. We also thank the ESRF staff for hospitality and support.**

**References:**

[1] S. Förster, K. Meinal, R. Hammer, M. Trautmann, and W. Widdra, Nature 502, 215 (2013)
[2] P. Stampfli, Helv. Phys. 59, 1260 (1986)
[3] F. Gähler, in: *Quasicrystalline Materials* (eds. E. D. Janot and J. M. Dubois), p. 272 (World Scientific, 1988)
[4] J. Kepler, Harmonices Mundi (Linz, 1619)
[5] S. Roy, R. Hammer, S. Förster, K. Mohseni, S. Nayak, H.L. Meyerheim, W. Hergert, and W. Widdra, unpublished