INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON



## **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	<b>Experiment title:</b> Temperature dependent X-ray diffraction measurements of decagonal Zn-Mg-Dy and Zn-Mg-Er quasicrystals	Experiment number: HC/798
Beamline:	Date of experiment:	Date of report:
BM01A	from: 10.04.2013 to: 12.04.2013	13.02.2014
Shifts:	Local contact(s):	Received at ESRF:
6	Vadim Diadkin	
Names and affiliations of applicants (* indicates experimentalists):		
Taylan Örs*		
Walter Steurer		
Thomas Weber		

### **Report:**

The findings of the mentioned experiment (together with the earlier experiment HS/4421) are reported in the following publication, which is recently accepted:

Ors, T., Takakura, H., Abe, E. & Steurer, W. (2014). Acta Cryst. B70, doi:10.1107/S2052520614001115.

## Abstract

A single crystal X-ray diffraction structure analysis of decagonal Zn-Mg-Dy, a Frank-Kaspertype quasicrystal, was performed using the higher-dimensional approach. For this first Frank-Kasper (F-K) decagonal quasicrystal studied so far, significant differences to the decagonal Al-TM (TM: transition metal) based phases were found. A new type of 2-fold occupation domain is located on certain edge centers of the five-dimensional (5D) unit cell. The structure can be described in terms of a two-cluster model based on a decagonal cluster ( $\approx$ 23 Å diameter) arranged on the vertices of a pentagon-Penrose tiling (PPT) and a star-like cluster covering the remaining space. This model is used for the 5D refinements, which converged to an R-value of 12.6%. The arrangement of clusters is significantly disordered as indicated by high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM). In order to check structure and stability at higher temperatures, in-situ high-temperature (HT) single crystal X-ray diffraction experiments were conducted at 598 K and 648 K (i.e. slightly below the decomposition temperature). The structure does not change significantly, however, the best quasiperiodic order is found at 598 K. The implication of these results on the stabilization mechanism of quasicrystals is discussed.