# EUROPEAN SYNCHROTRON RADIATION FACILITY

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 using the **Electronic Report Submission Application:** 

http://193.49.43.2:8080/smis/servlet/UserUtils?start

## Reports supporting requests for additional beam time

Reports can now 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:  Analysis of the structure of the (100) surface of fluorapatite as a function of different stages of hydration	Experiment number: SI - 1073
Beamline: ID03	<b>Date of experiment:</b> from: 01.12.2004 to: 07.12.2004	<b>Date of report</b> : 18.03.2007
Shifts: 21	Local contact(s): Dr. Ernesto Paiser	Received at ESRF:

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

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# **Report:**

This is resubmission of the report (dated 29.08.2005) which includes latest updates as on 18.03.07.

The experiment SI - 1073 was performed in ID03 beamline. We investigated the structure of the (100) fluorapatite surface with GIXRD techniques. In the first part of our beamtime at ESRF we measured specular and nonspecular CTRs of the fluorapatite surface in dry atmosphere. A large set of 12 symmetry independent CTRs was obtained from the integration of the measured rocking scans in dry environment.

In the second part of the experiment we measured specular (00L) and 9 non equivalent, nonspecular CTRs of the fluorapatite surface in humid environment.

Surface models for fluorapatite (100) surface in dry atmosphere and fluorapatite – water interface were obtained by data analysis in both cases.

The results from this experiment are successfully published in PHYSICAL REVIEW B 75, 035418 (2007). Below is the published abstract and complete list of references.

#### **Abstract:**

The structure of the fluorapatite (100) surface in humid ambient  $N_2$  with GIXRD is investigated and compared with results on the same surface in dry ambient conditions. Measurement of specular and non-specular crystal truncation rods (CTR) provided atomic scale information about the surface structure and the adsorption sites of the water molecules. In humid environment (75% r. h.), a laterally ordered monolayer of 4 water molecules per unit cell is formed at about 1.8 (1) Å above the relaxed surface reducing the magnitude of atomic relaxations observed on surface in dry conditions.

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# **References:**

- <sup>1</sup>S.Busch, U.Schwarz and R. Kniep, Chem., Mat., 13 (2001) 3260
- <sup>2</sup>M. Iijima, Y. Moriwaki, T. Takagi and J. Moradian-Oldak, J. Cryst. Growth, **222**, 615 (2001).
- <sup>3</sup>W.J. Landis, connect. Tissue Res. **35**, 1 (1996).
- <sup>4</sup>M. A. Fernandez-Seara, S. L. Wehrli, and F. W. Wehrli, Biophys. J. **82**, 522 (2002).
- <sup>5</sup>P. Fenter, N. C. Sturchio, Prog. Surf. Sci., **77**, 171 (2004)
- <sup>6</sup>D. Mkhonto, N. de Leeuw, J. Mat. Chem., **12**, 2633 (2002).
- <sup>7</sup>D. Zahn and O. Hochrein, Phys. Chem. Chem. Phys., **5**, 4004 (2003).
- <sup>8</sup>C. Park, P. Fenter, Z. Zhang, L. Cheng and N. C. Sturchio, Am. Mineralogist, **89**, 1647 (2004).
- <sup>9</sup>R. Feidenhans 1, Surf. Sci. Rep. **10**, 105 (1989).
- <sup>10</sup>J. Arsic, D. Kaminski, P. Poodt and E.Vlieg, Phys. Rev. B **69**, 245406 (2004)
- <sup>11</sup>M. F. Reedijk et. al., Phys. Rev. Lett., **90**, 066103-1 (2003)
- <sup>12</sup>I. K. Robinson, Acta Cryst. **A54**, 772 (1998) (and references therein).
- <sup>13</sup>J. Als-Nielson, Des McMorrow, *Elements of modern X-ray physics* (John Wiley & Sons Ltd., 2001) p.135.
- <sup>14</sup>S.Ferrer and F. Comin, Rev. Sci. Instrum. **66**, 1674 (1995).
- <sup>15</sup>U. Magdans, H. Gies, X. Torrelles and J. Rius, Eur. J. Mineral. 18, 83 (2006).
- <sup>16</sup>E. Vlieg, J. Appl.Crystallogr. **30**, 532 (1997).
- <sup>17</sup>E. Vlieg, J. Appl. Crystallogr. **33**, 401 (2000).
- <sup>18</sup>X. Torrelles, E. Barrena, C. Munuera, J. Rius, S. Ferrer and C. Ocal, Langmuir **20**, 9396 (2004).
- <sup>19</sup>J. M. Hughes, M. Cameron, K. D. Crowley, Am. Mineralogist, **74**, 870 (1989).
- <sup>20</sup>J. Arsic et al., J. Chem. Phys. **120**, 9720 (2004).