EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

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 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:** **Interaction of the (100) surface of fluorapatite with water and single amino acids gly and pro in solution.**	**Experiment number**: 25-02-603
Beamline: BM25B	**Date of experiment**: from: 22.02.2006 to: 28.02.2006	**Date of report**: 03.03.2008
Shifts:	**Local contact(s)**: Dr. German Rafael CASTRO	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

This is resubmission of the report (dated 23.03.2007) which includes latest updates as on 03.03.08.

The experiment 25-02-603 was performed at BM25-B Spline CRG beamline. We performed two separate GIXRD experiments to investigate the structure of (i) the fluorapatite – water interface (completely hydrated) (ii) fluorapatite - glycine interface. This experiment was a continuation of our previous measurements on fluorapatite (100) surface in dry and humid atmosphere [see ESRF Report SI-1073]. We investigated the structure of the (100) fluorapatite surface with a film of water by GIXRD techniques. Surface model for fluorapatite (100) – water interface was obtained by data analysis.

The results from this experiment are successfully published in Langmuir (2008) (Intended volume 6). Below is the published abstract.

Abstract:

The structure relaxation mechanism of the fluorapatite (100) surface under completely hydrated ambient conditions has been investigated with the grazing incidence X-ray diffraction (GIXRD) technique. Detailed information on lateral as well as perpendicular ordering corresponding to the water molecules and atomic relaxations of the (100) surface of fluorapatite (FAp) crystal was obtained from the experimental analysis of the CTR intensities. Two laterally ordered water layers are present at the water/mineral interface. The first layer consists of four water molecules located at 1.6(1) Å above the relaxed fluorapatite (100) surface while the second shows the presence of only two water molecules at a distance of 3.18(10) Å from the mineral surface. Thus, the first layer water molecules complete the truncated coordination sites of the topmost surface

Ca atoms, while the second water layer molecules remain bonded by means of H-bonding to the first layer molecules and the surface phosphate groups. Molecular mechanics simulations using force field techniques are in good agreement with this general structural behavior determined from the experiment.