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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 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.

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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:** **Structure of the multiferroic Fe/BaTiO3(001) interface**	**Experiment number**: SI-2224
Beamline: **ID03**	**Date of experiment**: from: 09/03/2011 to: 16/03/2011	**Date of report**:
Shifts: **18**	**Local contact(s)**: **Dr. Roberto FELICI**	*Received at ESRF:*

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Report:

We have successfully carried out the proposed surface x-ray diffraction experiments to analyze the structure of the Fe/$BaTiO_3$ (001) adsorption system. The experiments were carried out under ultra-high vacuum conditions at the beamline ID03.
In the first step we have prepared the $BaTiO_3$(001)-(2x1) surface reconstruction by repeated sputtering and annealing of a $BaTiO_3$ single crystal. Using the newly installed Maxipix area detector, we have collected intensities along both, integer order crystal truncation rods and fractional superlattice rods of the (2x1) reconstructed sample. For instance, Fig. 1 shows the (1/2 1 L) rod.

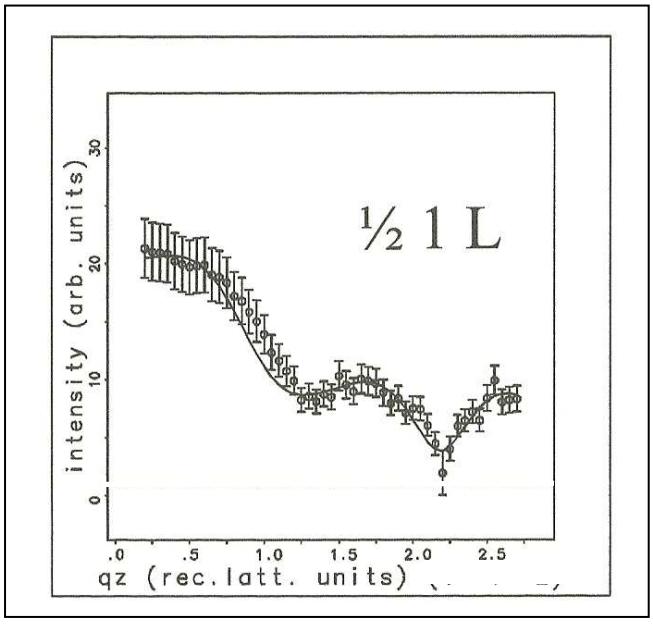

Fig. 1
Experimental (symbols) and calculated (lines) structure factor intensities, $|F|^2$, along the (1/2 1 L) superlattice rod of the (2x1) reconstructed $BaTiO_3$(001) surface.

Symbols represent experimental structure factors intensities ($|F|^2$). Standard deviations (1σ) derived from the counting statistics and the reproducibility of symmetry equivalent reflections are shown as error bars. The preliminary analysis by least squares fitting including all reflections provides evidence for a structure model, which is characterized by the presence of two terminating TiO_2 layers, very similar to the structure model previously proposed for $SrTiO_3$(001) [1-3].

In the second experiment we have deposited Fe on the $BaTiO_3$(001) surface, while the intensity at the (1 0 0.5) (anti-phase) reflection along the 10L crystal truncation rod of the $BaTiO_3$ (001) surface was monitored simultaneously. This is shown in Fig.2.

The arrows indicate the time at which the shutter was opened and closed, respectively. The total amount of Fe deposited equals to an equivalent of about 17 monolayers (ML) when referenced to the atom number density of the Fe(001) surface (1 ML: 1.21×10^{15} atoms/cm^2). Fe-deposition does not lead to a significant modulation of the CTR intensity which is expected if coherent epitaxial growth of Fe on a specific site of the single crystalline $BaTiO_3$ surface is assumed [4]. Rather, we observe a slow and continuous drop of intensity which can be interpreted by disordered growth of Fe. After about 3-4 ML coverage the decay rate increases, which might be attributed to the completion of a closed Fe-adlayer.

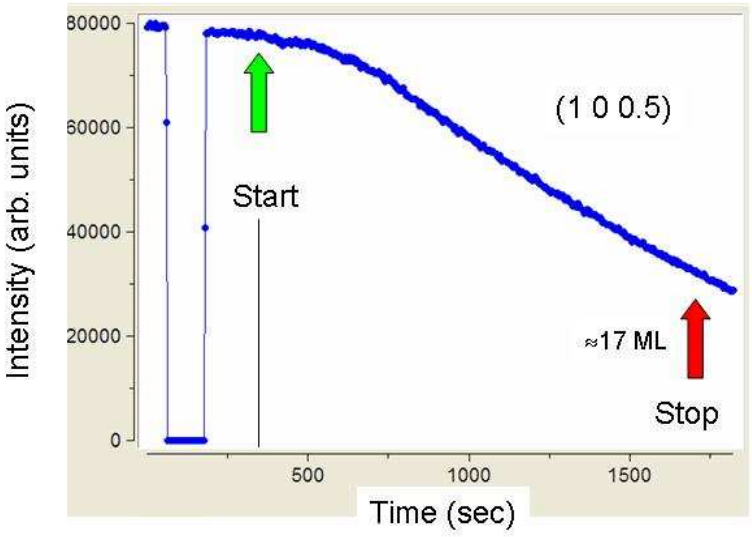

Fig. 2
Evolution of the (10 0.5) anti-phase reflection intensity during Fe deposition. Arrows mark start and stop of deposition. The total amount of Fe deposited equals to about 17 ML [referenced to the Fe(001) surface atom number density].

References:

[1] N. Erdman,K.R. Poeppelmeier, M. Asta, O. Warschkow, D. Ellis, and L.D. Marks, Nature 419, 55 (2002)
[2] R. Herger, P.R. Willmott, O. Bunk, C.M. Schlepütz, B.D. Patterson, and B. Delley, Phys. Rev. Lett. 98, 076102 (2007)
[3] N. Iles, F. Finocchi, and K.D. Khodja, J. Phys. Cond. Matter 22, 1 (2010)
[4] M. Fechner, I.V. Maznichenko, S. Ostanin, A. Ernst, J. Henk, P. Bruno, and I. Mertig, Phys. Rev. B. 78, 212406 (2008)