EUROPEAN **S**YNCHROTRON **R**ADIATION **F**ACILITY

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:** **Structure of the Fe/O/Fe(001)-p(1x1) surfactant system**	**Experiment number**: SI-2039
Beamline: **ID03**	**Date of experiment**: from: 02/06/2012 to: 05/06/2012	**Date of report**:
Shifts: **18**	**Local contact(s)**: **Dr. Roberto FELICI**	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

(1) H. L. MEYERHEIM *(MPI f. Mikrostrukturphysik, D-06120 Halle (Germany)
(2) K. MOHSENI (MPI-Halle)*
(3) N. JEDRECY (Univ. Paris VI)*
(4) W. FENG (MPI Halle)*
(5) J. KIRSCHNER (MPI-Halle)

Report:

It was the aim of the experiments to prepare the O/Fe(001)-p(1x1) structure and to deposit different amounts of Fe on this surface (0.25, 0.50, 1.00, 1.50 ML) to study the coverage dependent atomic geometry of this surfactant system. The experiments could be carried out succesfully. Thanks to the fast data collection by using a two dimensional pixel detector we have collected eight independent data sets each consisting of about 600 reflections along 15 truncation rods reducing to

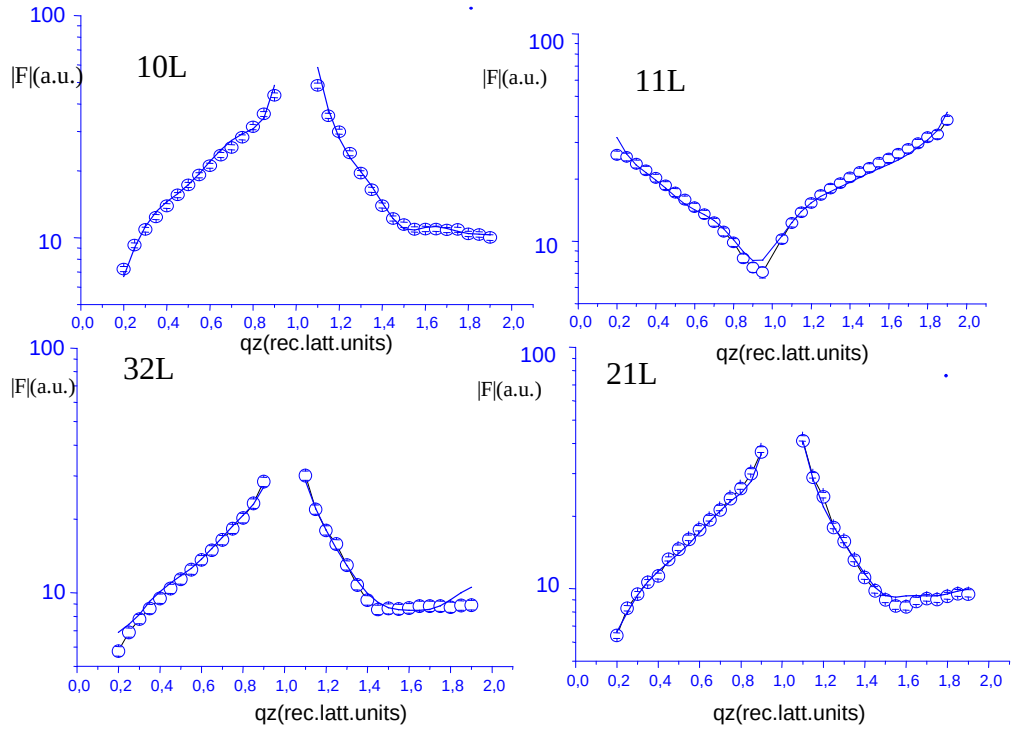

Fig. 1 Experimental (symbols) and calculated (lines) structure factor amplitudes for 0.5 ML Fe on O/Fe(001)-p(1x1). Only four out of eight CTRs are shown.

about 300 symmetry independent reflections along eight crystal truncation rods (CTRs). Fig. 1 shows as a representative example the experimental (symbols) structure factor amplitudes (|F|) along four CTRs for the sample where 0.5 ML Fe were deposited.
Solid lines represent the calculated |F| which is related to the structure model shown in Fig.2. Even by direct inspection the excellent fit quality is evident.

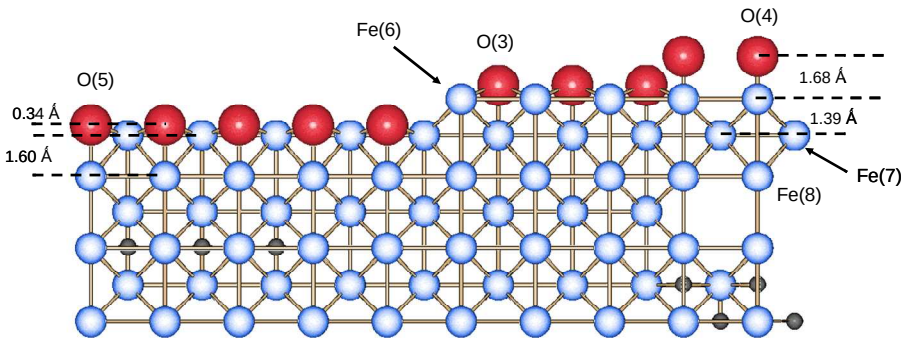

Fig. 2 Structure model for 0.5 ML Fe on O/Fe(001)-p(1x1). Oxygen and Fe-atoms are shown as red (large) and blue (small) spheres. The number in each layer approx. represents the fractional coverage. Distances are given in Ångstrom units.

On a quantitative basis, the fit quality is measured by the unweighted residuum (Ru), which for all data sets lies in the range between Ru=4.5 and 6.0%, corresponding to a goodness of fit (GOF) of GOF=1.7 to 2.5, respectively.
In detail, we find that there is some fraction of oxygen atoms (red balls [O(4)]) located on top of the Fe-atoms (6) forming the growing layer on the complete Fe layer (7) under neath. The remaining O-atoms (5 and 3) on the original and the growing layer (7 and 6) are located in "conventional" hollow sites as previsously derived on the basis of LEED and SXRD analyses [1,2]. The number of Fe(6) atoms in Fig.2 represents the coverage only. STM images indicate that the size of the Fe(6) islands is of the order of about 1nm. Ab initio calculations are currently carried out to investigate the correlation of the island size and with it the effect of the mesoscopic misfit [3] with the presence of two different oxygen adsorption sites. Our findings might explain the observation of a periodically modulated surface magnetic moment previously found by second harmonic generation [4]

References:

[1] K.O. Legg, F. Jona, D.W. Jepsen, and P.M. Marcus, Phys. Rev. B 16, 5271 (1977)
[2] S.S. Parihar, H. L. Meyerheim, K. Mohseni, S. Ostanin, A. Ernst, N. Jedrecy, R. Felici, and J. Kirschner, Phys. Rev. B 81, 075428 (2010)
[3] O. Mironets, H.L. Meyerheim, C. Tusche, V.S. Stepanyuk, E. Soyka, P. Zschack, H. Hong, N. Jeutter, R. Felici, and J. Kirschner, Phys. Rev. Lett. 100, 096103 (2008)
[4] M. Nyvlt, F. Bisio, J. Franta, C.L. Gao, H. Petek, and J. Kirschner, Phys. Rev. Lett. 95, 127201 (2005)