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:** **Surface x-ray diffraction study of the structure of O/Fe(001)-p(1×1)**	**Experiment number**: SI-1848
Beamline: **ID03**	**Date of experiment**: from: 11/03/2009 to: 18/03/2009	**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) S. S. PARIHAR (MPI-Halle)*
(3) K. MOHSENI (MPI-Halle)*
(3) N. JEDRECY (Univ. Paris VI)*
(4) J. KIRSCHNER (MPI-Halle)

Report:

We have carried out a highly precise surface x-ray diffraction (SXRD) study on the geometric structure of the O/Fe(001)-p(1×1) system, for which controversy exists even more than 30 years after its first investigation [1-3].

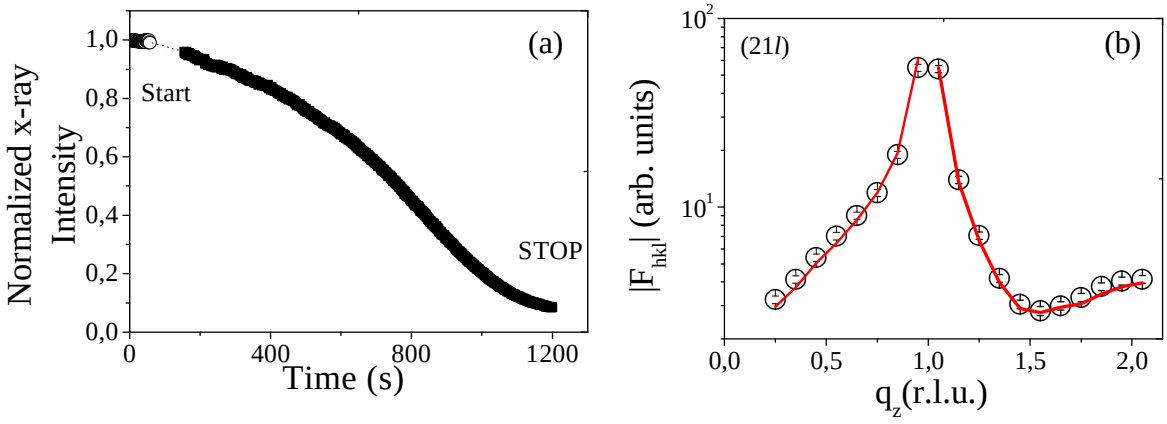

Fig. 1: (a) Anti-phase (1 0 0.1) reflection intensity versus oxygen dosing ($pO_2 \approx 5x10^{-9}$mbar). The total dosage equals to about 4.2 Langmuirs.
(b) Experimental (symbols) and calculated (lines) structure factor $|F_{hkl}|$ amplitudes along q_z for the (21L). In total 9 CTRs corresponding to 180 symmetry independent reflections were measured.

The saturation of the CTR intensity after about 1100 seconds of dosing (≈4.2 Langmuirs) corresponds to about 1 ML of oxygen. For this sample the SXRD analysis

indicates the formation of FeO-like islands three layers thick and roughening of the Fe(001) surface [4]. After annealing at about 500°C for one minute the surface flattens and a well ordered structure is formed. On the basis of 180 symmetry independent SXRD reflections a model structure is derived, which is shown in side view in Fig.2(a).

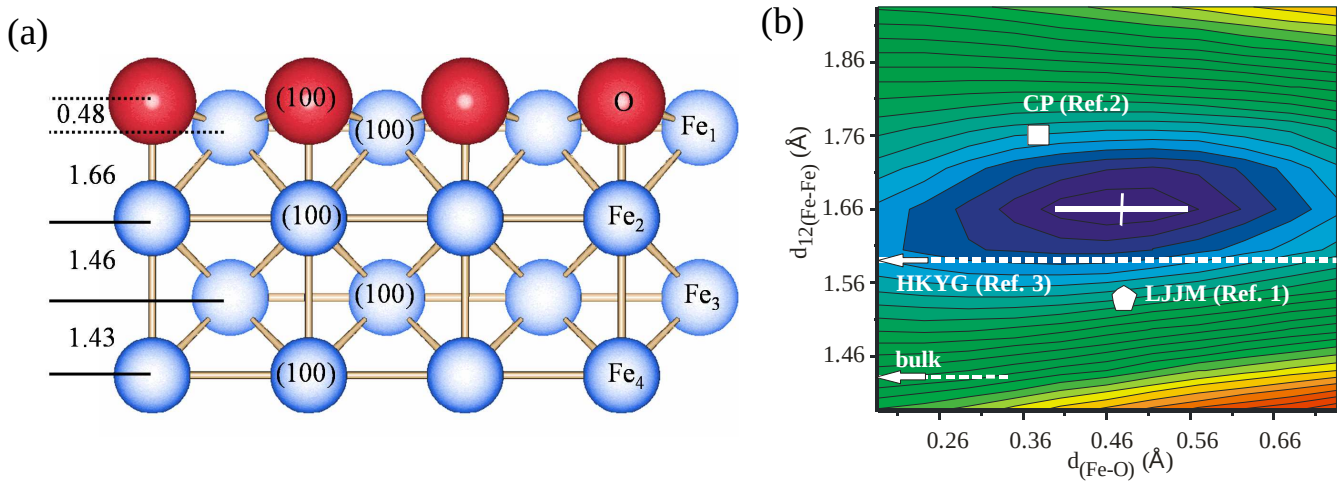

Fig. 2: (a) Structure model for O/Fe(001)-p(1×1) in side view. Blue and red balls represent Fe- and O-atoms, respectively. Distances are listed on the left in Angstrom units. Layers are fully occupied (100%). (b): Contour plot of Ru vs. top layer spacing d_{12}, and oxygen adsorption height d_O. Best fit (cross) corresponds to Ru=0.05, the contour level spacing is ΔRu=0.01. The width of the cross corresponds to the estimated error bars based on the variation of Ru. Symbols and dashed lines indicate results of previous studies (see Refs. [1-3]).

Oxygen atoms in hollow sites reside at d_O =0.48 (5) Å above the top layer Fe-atoms (Fe_1), the first Fe-Fe interlayer distance d_{12} equals to 1.66(2) Å, corresponding to a 16% expansion relative to the bulk spacing (1.43 Å). The refinement of the oxygen occupancy yields Θ=1.1(2), indicating a fully occupied surface layer (not shown) [4]. The variation of the unweighted residuum (Ru) versus d_O and d_{12} is shown in Fig. 2(b). The best fit value (indicated by the cross at the minimum) corresponds to Ru=0.05, which is an excellent value for SXRD studies. With regard to d_{12} our analysis is at variance with previous studies [1-3]. Differences might be attributed to the sensitivity of d_{12} on the total oxygen occupancy [4]. Our study is the most accurate one carried out so far for this system.

References

[1] K.O. Legg, F. Jona, D. W. Jespen, and P. M. Marcus, Phys. Rev. B 16, 5271 (1977)
[2] S. R. Chubb, and W. E. Pickett, Phys. Rev. Lett. 58, 1248 (1987)
[3] R.L. Headrick, P. Konarski, S.M. Yalisove, and W.R. Graham, Phys. Rev. B 39, 5713 (1989)
[4] S.S. Parihar, H.L. Meyerheim, K. Mohseni, N. Jedrecy, S. Ostanin, A. Ernst, R. Felici, and J. Kirschner, unpublished