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.

Report:
We have successfully carried out the proposed surface x-ray diffraction experiments on the structure of the Fe/O/Fe(001) surfactant system. In the following we report on some results of our experiments, a detailed publication will follow:

Fig. 1(a)

Fig. 1(a): Normalized x-ray intensity close to the (100) antiphase condition during oxygen deposition on Fe(001). The red and green arrow indicate start and stop of dosing. Saturation is at 10% of the initial value. Intensity is recovered to 50% by annealing indicating the formation of the ordered O/Fe(001)-p(1x1) structure. The inset shows the x-ray intensity variation during Fe deposition on O/Fe(001)-p(1×1).

(b): Experimental (symbols) and calculated (lines) structure factor amplitudes ($|F_{hkl}|$) along the (11l) and (21l) crystal truncation rod after dosing 0.5ML Fe on O/Fe(001)-p(1x1)

It was the aim of this experiment to analyze in detail the structure of the "surfactant" system Fe/O/Fe(001)-p(1x1). First, the O/Fe(001)-p(1x1) structure was prepared by dosing oxygen at $p(O_2)= 9\times10^{-9}$ mbar until saturation of the (100) anti-phase condition is observed at about 10% of the original value (I_0) (see Fig.1a). Annealing at 500°C for 1 min. leads to the recovery of I_0 to 50%, which is related to formation of the ordered O/Fe(001)-p(1×1) structure [1].

Subsequently, Fe was added under ultra-high vaccum (UHV) conditions and at different oxygen partial pressures. For instance, the inset in Fig.1a shows the (100) reflection intensity during deposition of 0.5 ML Fe on O/Fe(001)-p(1×1) in UHV. It continuously drops to a minimum about 50% of the initial value.

After preparation about 200 reflections were collected along seven crystal truncation rods (CTRs) averaging to 135 by symmetry equivalence. In Fig. 1(b) the best fit (solid lines) for two rods is shown corresponding to an overall $R_u=0.09$ and GOF=1.35.
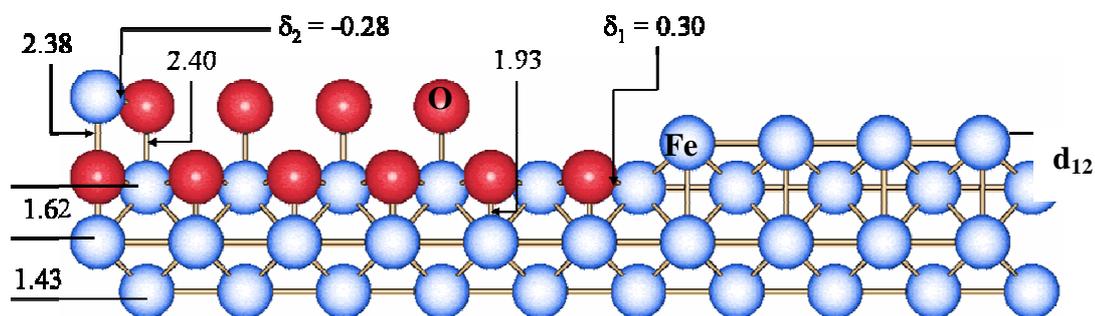
Fig. 2 Structure model for 0.5 ML Fe on O/Fe(001)-p(1×1) in side view. Blue and red balls represent Fe- and O-atoms, respectively. Distances are in Angstrom units. Parameter δ repressnts the height difference between O and Fe-atoms.

In general, we find complex structures, which are at variance with simple surfactant models assumed so far. In the case of 0.5 ML Fe on O/Fe(001), which corresponds to the first minimum of the (100) CTR intensity as well as in previous medium energy electron diffraction experiments [2], we find that approximately 0.4 ML of Fe is grown as bcc Fe on Fe(001) at a contracted distance d_{12}, while the remaining part of the surface can be characterized by a local FeO type structure. Most importantly, our model provides an explanation for the so far unresolved observations of the oscillatory behaviour of the magnetic second harmonic generation (SHG) signal with Fe coverage, where minima and maxima were found at half and full layer coverage, respectively [2]. Dosing under oxygen partial prsssures in the 10^{-8} mbar range in general leads to the formation of FeO like islands several layers thick.

References:

[1] 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).
[2] M. Nyvlt, F. Bisio, J. Franta, C. L. Gao, H. Petek, and J. Kirschner, Phys. Rev. Lett. 95, 12720 (1999)