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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	**X-ray analysis of the geometric structure and interface homogeneity of the ZnO/Fe(110) interface**	**Experiment number**: SI-1687
Beamline: ID32	**Date of experiment**: from: 8.4.2008 to: 17.4.2008	**Date of report**:
Shifts: 24	**Local contact(s)**: Dr Juan RUBIO-ZUAZO	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

(1) H. L. Meyerheim *(MPI f. Mikrostrukturphysik, D-06120 Halle (Germany)

(2) German CASTRO (ESRF)*

(3) Nathalie JEDRECY (Univ. Paris VI)*

(4) Jürgen KIRSCHNER (MPI-Halle)

(5) Katayoon MOHSENI (MPI-Halle)*

(6) Christian TUSCHE (MPI-Halle)

Report:

We have proposed a surface x-ray diffraction (SXRD) study of the geometric structure of ultrathin ZnO films deposited by electron beam evaporation on Fe(/110). The proposed experiments could be carried out successfully. Two samples covered by 3 and 6 ML ZnO were prepared

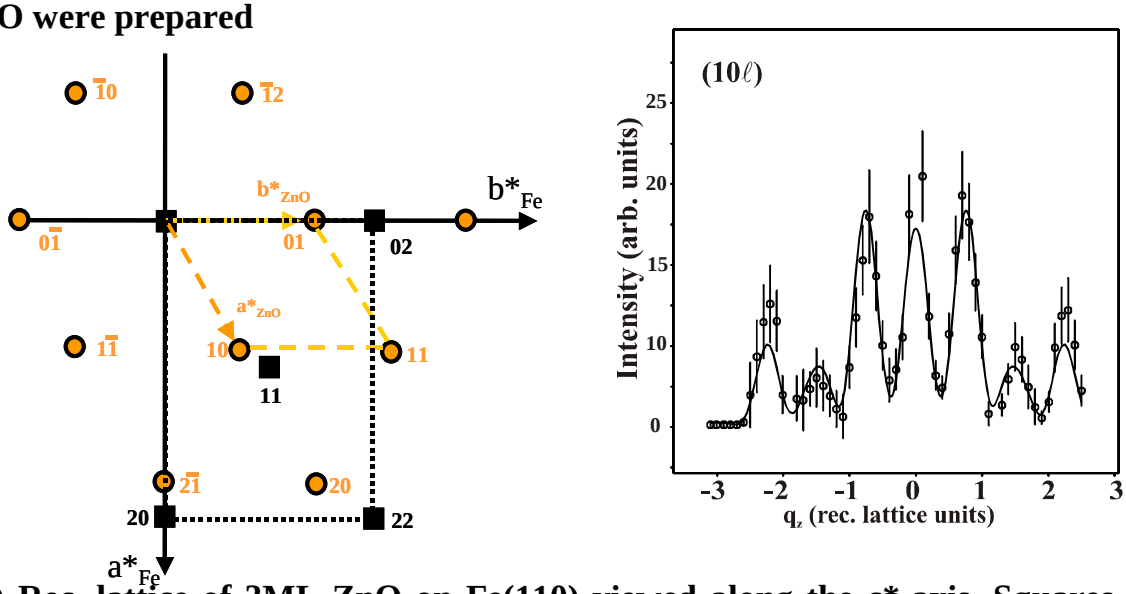

Fig.1: (a) Rec. lattice of 3ML ZnO on Fe(110) viewed along the c*-axis. Squares and circles correspond to rods of the Fe-substrate and the ZnO-overlayer, respectively. (b) Measured (symbols) and calculated (line) intensities along the ZnO (10L) rod. Reflection indexes refer to the individual lattices.

From the positions of the ZnO-rods in the a*-b*-plane of the reciprocal space [circles, see Fig. 1(a)] the ZnO-overlayers were found to be incommensurate with the Fe(110) lattice (solid squares) by adopting the bulk lattice constant a=b=3.249Å to within 0.005 Å.

Reflection intensities were collected along several ZnO and Fe(110) rods. Fig. 1(b) shows for the 3ML sample the measured intensity distribution along the (10L) ZnO-rod (symbols) together with the intensities (line) calculated for the structure model outlined in Fig. (2). High quality fits can be achieved quantified by the Goodness of Fit (GOF) in the 0.9 range, while the unweighted residual is in the 0.2 regime (based on intensities).

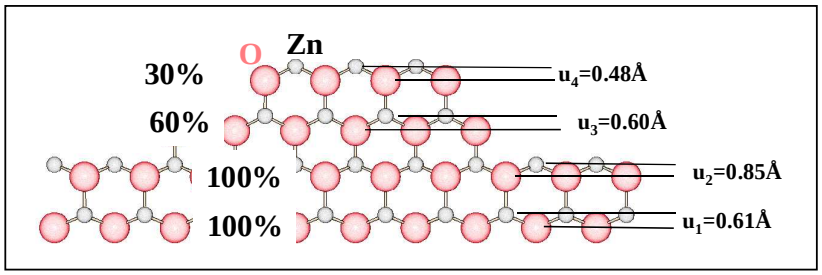

Fig.2 : Structure model for 3ML ZnO on Fe(110).

The 3ML adlayer is characterized by a bulk like ZnO structure, i.e. there is no relaxation of the Wurtzite structure to the h-BN-type structure as observed for ZnO/Ag(111) for the first two layers adjacent to the Ag(111) surface [1]. We have carried out extensive systematic calculations varying all parameters u_1 to u_4 characterizing the structure type (u=0.0 Å and u=0.63 Å corresponding to the h-BN and the bulk Wurtzite structure, respectively). As an example Fig. 3 shows the contour plot of the GOF versus u_1 and u_2 keeping u_3 and u_4 at the optimum values (0.60 and 0.48Å, respectively). The GOF minimum (see cross) is found for u_1=0.61 Å and u_2=0.85 Å. Although the first has an error bar in the 0.1-0.2 Å range, values below about 0.5 Å can clearly be ruled out.

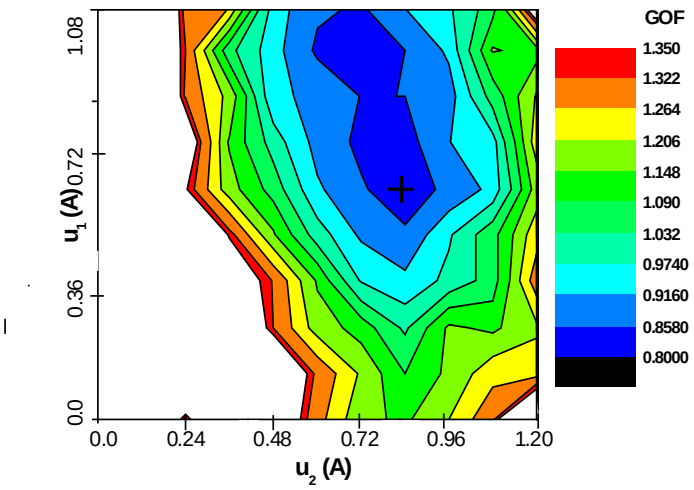

Fig.3: Contour plot of GOF vs. u_1 and u_2. The cross indicates the minimum.

The layer-occupancies were derived to 100%, 100%, 60% and 30% leading to a total coverage of 2.9 atomic layers. This is at some variance with the film thickness of 3.8±0.8Å (≈2 complete layers) derived from high energy photoemission spectroscopy (primary beam energy=14keV) using extra-polated values for the absorption cross sections of Zn and Fe [2].

The analysis of the Fe(110) truncation rods reveals that the surface is covered by a substantial amount (≈0.8-1 ML) of oxygen, consistent with previous photoelectron spectroscopy ex-periments

References:

[1] C. Tusche, H. L. Meyerheim, and J. Kirschner, Phys. Rev. Lett. 99, 026102 (2007)

[2] Trzhaskovskaya et al. Atomic Data &Nucl. Data Tables 77, 97 (2001)