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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.

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 and surface depolarization of Cobalt doped ZnO in the ultra thin film limit**	**Experiment number**: SI-1641
Beamline: ID32	**Date of experiment**: from: 30.10.2007 to: 6.11.2007	**Date of report**:
Shifts: 21	**Local contact(s)**: Dr. Jerome Roy	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

(1) H. L. Meyerheim *(Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Germany)

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(3) J. Kirschner [affiliation as (1)]

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(5) F. Yildiz [affiliation as (1)]

Report:

It was the aim of the experiment to study the structure of ultrathin Zn(1-x)Co(x)O films deposited on Ag(111) by pulsed laser depoition (PLD) using surface x-ray diffraction (SXRD). The proposed experiments were carried out successfully.
Several samples in the coverage range between about 2 and 6 monolayers (ML) were prepared in the surface characterization laboratory (SCL). Auger electron spectroscopy indicated a dopant concentration of the Co-atoms (x) in the 25-30% range.

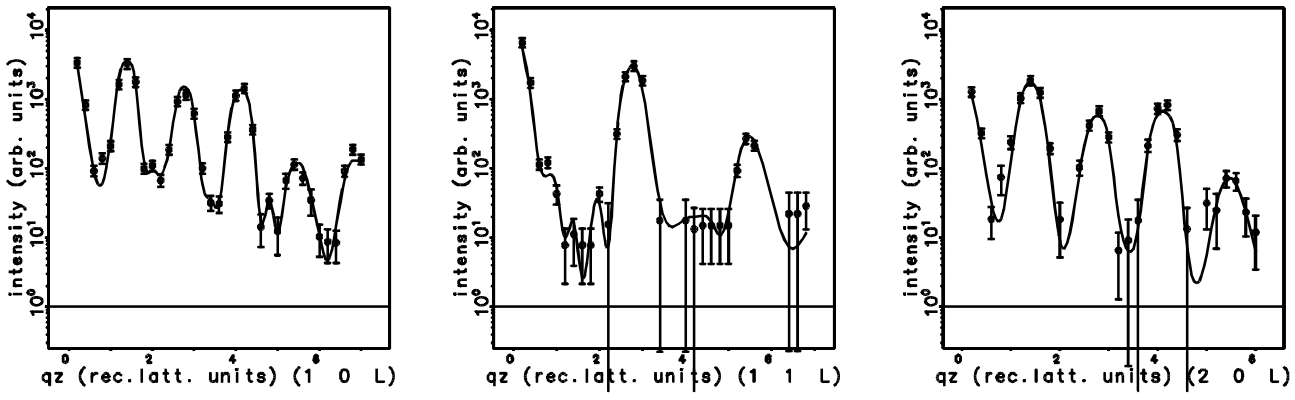

Fig.1: Data (symbols) and fits (lines) for 5ML Zn(Co)O/Ag(111) along three out of five symmetry independent rods.

After sample transfer to the ID32 beamline, SXRD intensities were collected. The Zn(Co)O films adopt an incommensurate structure relative to the Ag(111) surface with in-plane lattice constants about one percent lower than 3.303(2) Å measured for pure ZnO-films [1].

As a representative example, Fig. (1) shows the measured (symbols) and calculated (lines) intensities along some symmetry independent rods for 5ML Zn(Co)O/Ag(111). Highly accurate fits could be achieved by assuming a structrure model schematically outlined in Fig. (2).

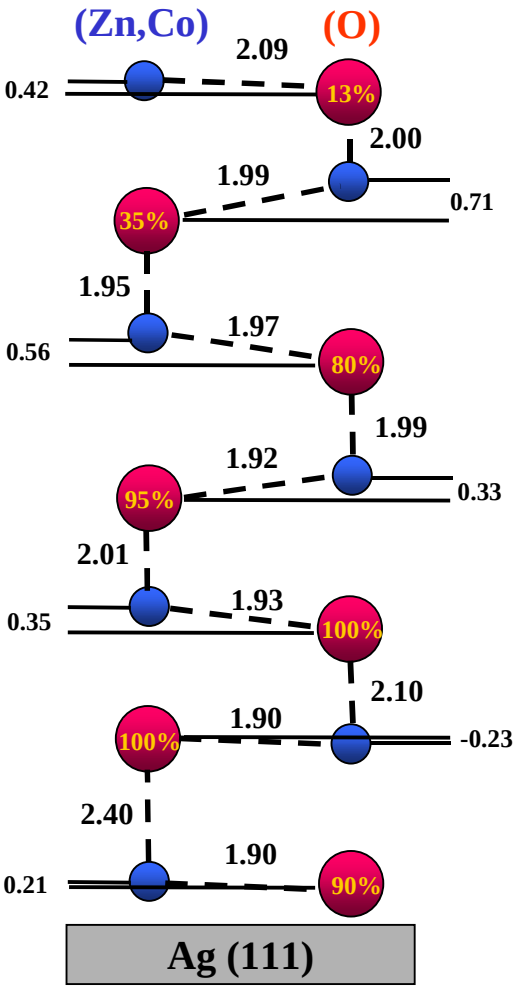

Fig.2 Structure model for 5 ML Zn(Co)O deposited on Ag(111).

Zn (Co) and oxygen atoms are represented by small and large circles, respectively. The occupancy in percent of a ML within each layer is indicated within the spheres representing the oxygen atoms. Within each layer the 1:1 metal to oxygen stoichiometry is preserved. Distances are given in Ångström units (with an error bar of about 0.10 Å).

Similar to pure ZnO-layers on Ag(111), [1], Zn(Co)O adopts a planar Boron-Nitride-type structure within the first two layers. Here, the vertical spacing between the oxygen and the metal atoms is considerably reduced as compared to the bulk value of 0.65 Å. Simultaneously there is a strong anisotropy in the bond length (in-plane: 1.90 Å, out of plane: 2.10-2.40 Å). Within the upper layers there is a transition to the bulk ZnO Wurtzite–type structure. In addition, a proper fit like that shown in Fig.1 requires the consideration of a very strong anisotropy of the atomic (static) displacements characterized by a large enhancement along the normal direction within the first two layers including anharmonic terms [2]. The data analysis is still in progress.

References:

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

[2] W. F. Kuhs, Acta Cryst. A48, 80 (1992)