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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:** Investigation of the crystallography and stoichiometry depth profile of metal oxide-semiconductor Schottky barriers by HAXPES in combination with Surface X-ray diffraction	**Experiment number**: HE-3605
Beamline: BM25B	**Date of experiment**: from: 11/03/11 to: 16/03/11	**Date of report**: 2/28/2012
Shifts: 15	**Local contact(s)**: Juan Rubio-Zuazo	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Alexander Lajn *[a]
Michael Lorenz *[a]
Friedrich Schein *[a]
Dr. German r. Castro [b]

[a]Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik
Linnéstraße 5, 04103 Leipzig, Germany
Tel: 0049 341 97 32 753, Fax: 0049 341 97 32 668
mail: lajn@uni-leipzig.de
www: www.uni-leipzig.de/~hlp, www.uni-leipzig.de/~lajn

[b]Spanish CRG BM25 Beamline - SpLine
European Synchrotron Radiation Facility
6, Rue Jules Horowitz BP 220 F-38043 Grenoble Cedex 09 FRANCE

Aim of the experiment

Primary aim of this experiment was to determine a depth profile of the oxidational state of noble metal films, which were deposited in oxidizing environment. In order to be able to link the depth profile to the exact sample structure, X-ray reflectivity measurements were planned.

Sample description:

For the experiment HE-3605, four different thin films were prepared on previously annealed hydrothermally-grown oxygen-terminated c-ZnO substrates (purchased from Crystec). Subsequently, films were deposited using DC magnetron sputtering of Au and Pt. For each metal, one film was deposited in argon atmosphere and one film in a mixed argon/oxygen – atmosphere. The deposition conditions were adapted, such that the thickness of the all thin films was about 20 nm.

Measurement conditions:

Generally, all measurements could be comfortably performed and the local contacts supported the work satisfactorily.

Obtained Results:

For each sample, the zinc $L_1$2s-level was measured. Furthermore, for each metal one core level was measured. The beam energy was varied between 9 keV and 16 keV. In the following the results obtained for the Pt grown in oxidizing conditions are sketched.

From the XRR spectrum, recorded at a photon energy of 9 keV, the thickness and the density of the overlayer film was extracted using the IMD extension of the XOP software package (cmp. fig. 1). The respective inelastic mean free path was calculated using the TPP-2M formula and the simulated depth dependence of the photoemission contribution reveals that the contribution of the interfacial region can be tuned by about a factor of three for the applied photon energy range.

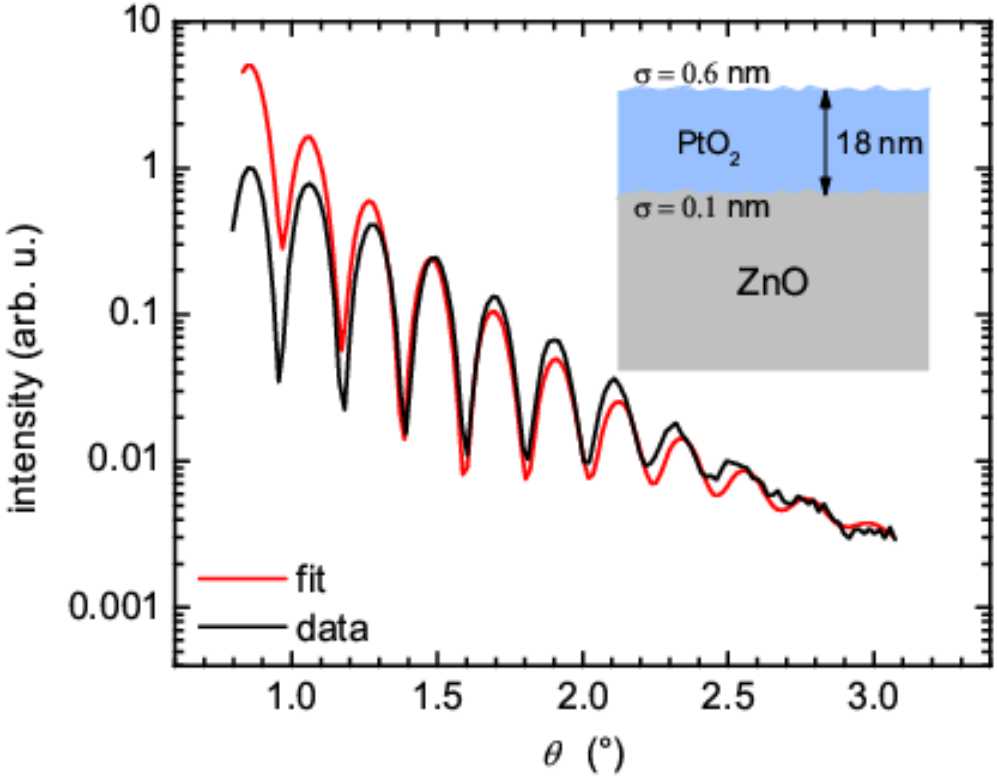

Figure 1: X-ray reflectivity measurement for film thickness determination at a beam energy of 9 keV (λ=1.38 Å). The inset depicts the assumed layer stack model and the resulting fit parameters.

The core level spectra of the overlayer, corrected by a fitted background (using UNIFIT 2011 software) are depicted in fig. 3a). Here, the photon energy was already corrected with the spectral position of the substrate core level. Luckily, the Zn exhibits a very low chemical shift, making the possible changing degree of oxidation of the Zn within the substrate unimportant. The peak position is obviously neither constant nor monotonically shifting with changing beam energy, which indicates a remaining charging effect for some samples. Therefore, for the following fitting procedure, the spectral position of the Pt^0 $3d_{3/2}$ core level has to remain as free fitting parameter. Generally, the overlayer spectra are fitted with a combination of 3 Voigt profiles, representing the known Pt oxidational states: Pt^0, Pt^{+2} and Pt^{+4}. The resulting energetic position of the Pt^0 level is depicted in fig. 3b), reproducing the

already mentioned uncertainty in the calibration of the photon energy. From the peak areas of the components, the fraction of the respective oxidational state can be calculated.

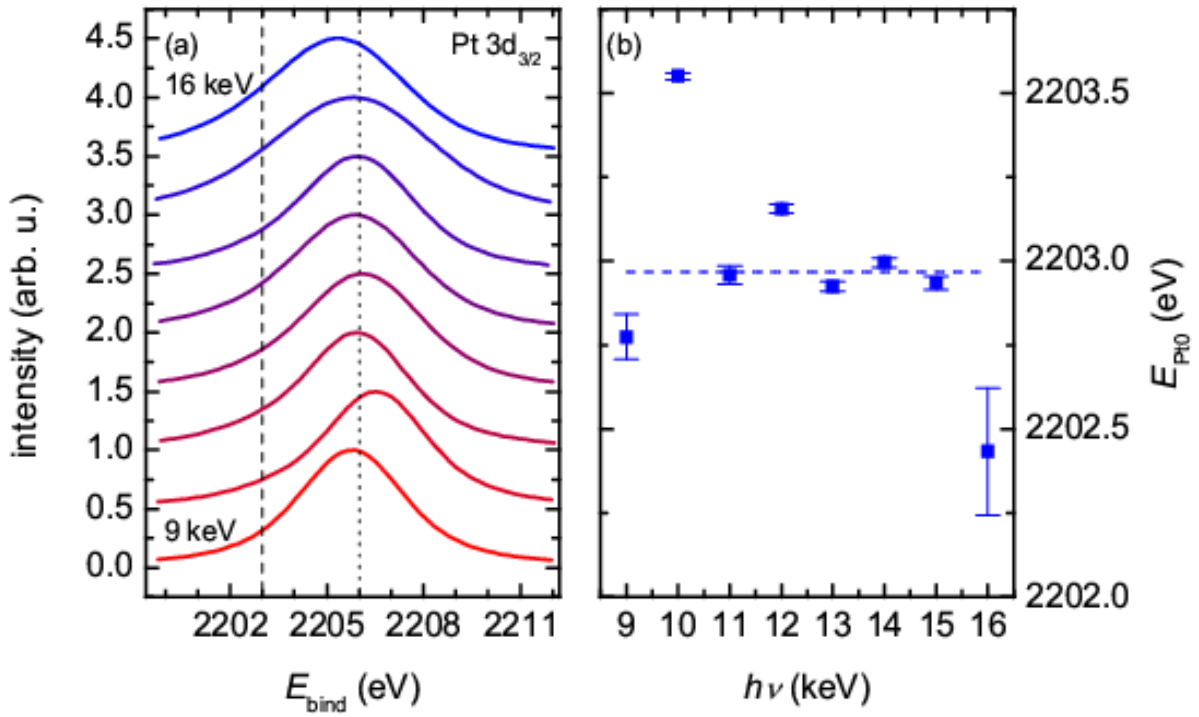

Figure 3: (a) Background-corrected and normalized spectra of the Pt core level recorded for different beam energies (shifted for clarity). The dashed line indicates the mean position of the Pt^0 level and the dotted line the mean position of the Pt^{-2} level. (b) Spectral position of the Pt^0 $3d_{3/2}$ core level as extracted from the peak fitting. The dashed line indicates the mean value.

Conclusion

In summary, the experiment was successfull in terms of the determination of the depth profile of the oxidational state of reactively sputtered platinum on zinc oxide substrates. Thus, a valuable insight into the functionality of rectifying contacts to zinc oxide was gained.