Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

Supplementary Information - "Thermodynamic Stability and Control of Oxygen Reactivity at Functional Oxide Interfaces: EuO on ITO"

Timm Gerber,[a,#] Patrick Lömker,[a] Bernardus Zijlstra,[a] Claire Besson,[b,‡] David Müller,[a] Willi Zander,[c] Jürgen Schubert,[c] Mihaela Gorgoi,[d] and Martina Müller [a,e,*]

Received Date
Accepted Date

DOI: 10.1039/xxxxxxxxxx

www.rsc.org/journalname

1 Eu Distillation Condition

Fig. 1 shows HAXPES data of a sample grown under the Eu distillation condition i. e. 4 nm EuO/ITO with the EuO layer grown at T_S =400 °C with $J_{Eu}/J_O = 2$. The sample is largely over-oxidized, similar to sample type (i) discussed in the manuscript.

2 Chemical Stability of the YSZ Buffer Layer

In order to investigate the chemical stability of the YSZ buffer layer in sample type (ii), we recorded HAXPES data of the Zr 3*d* core level. The spectra are depicted in Fig. 2. For all photon energies, we find that the two components of the Zr 3*d* doublet are located at 182.9 eV and 185.3 eV, which is the expected binding energy for YSZ[1]. No other peaks are observed, especially none at 178.8 eV which would be characteristic for metallic Zr^0. We conclude that the buffer layer is homogeneous and stable against reduction by the EuO layer.

[a] *Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Jülich, Germany*
[b] *Institut für Anorganische Chemie, RWTH Aachen University, Germany*
‡ *Present address: Department of Chemistry, George Washington University, Washington, District Of Columbia, United States*
[c] *Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, Jülich, Germany*
[d] *Helmholtz-Zentrum für Materialien und Energie GmbH, Berlin, Germany*
[e] *Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany*
[#] *E-mail: t.gerber@fz-juelich.de*
[*] *E-mail: mart.mueller@fz-juelich.de*

3 Fitting Procedures

Exemplary fits of Eu 3*d* and In 3*d* spectra are shown in Fig. 3 and Fig. 4. Both core levels show spin-orbit splitting into $3d_{5/2}$ and $3d_{3/2}$ components. The Eu 3*d* spectrum in Fig. 3 is fitted with components for divalent Eu^{2+} (orange, the signature of stoichiometric EuO) and trivalent Eu^{3+} (brown, the signature of over-oxidized phases). Further, plasmonic excitations in the Al capping layer cause satellite peaks (gray) which are shifted by 16 eV with respect to the peak they originate from. The Eu^{2+} component is fitted with a complex multiplet structure[2]. Details of the fitting procedure are describe in[3].

The In 3*d* spectrum in Fig. 4 is also spin-orbit split into $3d_{5/2}$ and $3d_{3/2}$. It is fitted with the following components: one located at 444.9 eV, which denotes trivalent In^{3+} (as expected for Sn:In_2O_3)[4], a second component located at 445.7 eV which can be attributed to screening effects caused by the Sn dopants[5], and a third component located at 443.9 eV which is characteristic for metallic In^0.

References

1 H. Behner, J. Wecker, T. Matthée and K. Samwer, *Surf. Interface Anal.*, 1992, **18**, 685–690.
2 E.-J. Cho, S.-J. Oh, S. Imada, S. Suga, T. Suzuki and T. Kasuya, *Phys. Rev. B*, 1995, **51**, 10146–10149.
3 C. Caspers, M. Müller, A. X. Gray, A. M. Kaiser, A. Gloskovskii, C. S. Fadley, W. Drube and C. M. Schneider, *Phys. Rev. B*, 2011, **84**, 205217.
4 M. Burgener and A. Goldmann, *Surf. Sci.*, 2003, **540**, 89–96.
5 V. Christou, M. Etchells, O. Renault, P. J. Dobson, O. V. Salata, G. Beamson and R. G. Egdell, *J. Appl. Phys.*, 2000, **88**, 5180–5187.

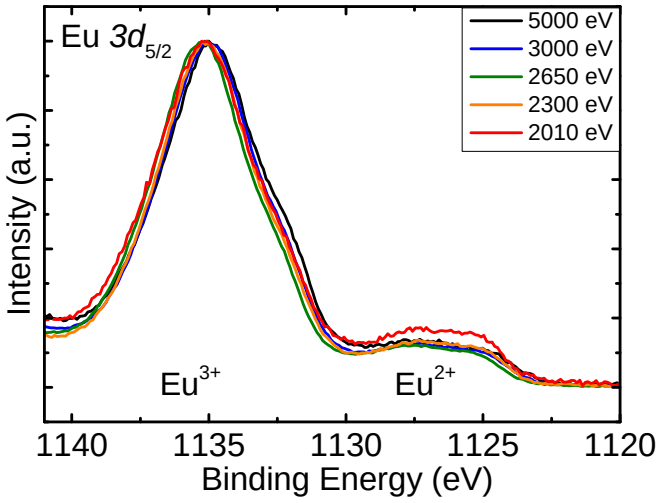

Fig. 1 HAXPES spectra of the Eu $3d_{5/2}$ core level of a sample grown under the Eu distillation condition. Spectra normalized to the Eu^{3+} component.

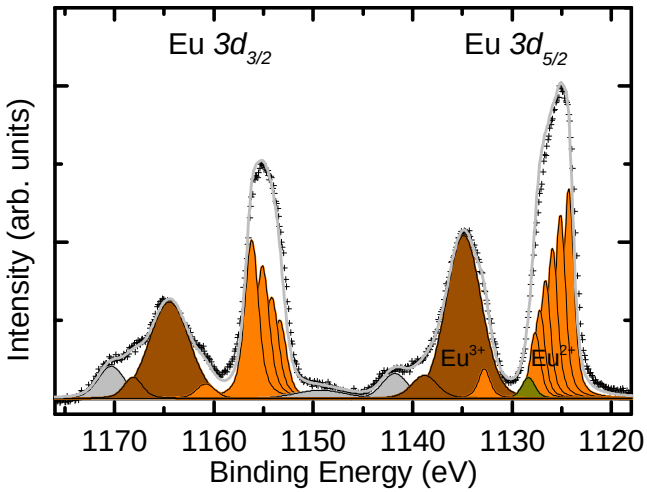

Fig. 3 HAXPES spectrum of the Eu $3d$ core level of sample type (iii). Spectrum recorded with a photon energy of $5000\,\mathrm{eV}$. Eu^{2+} components are shown in orange, Eu^{3+} in brown, and plasmonic excitation in gray. Black crosses represent the experimental data, gray line is the superposition of all fit components.

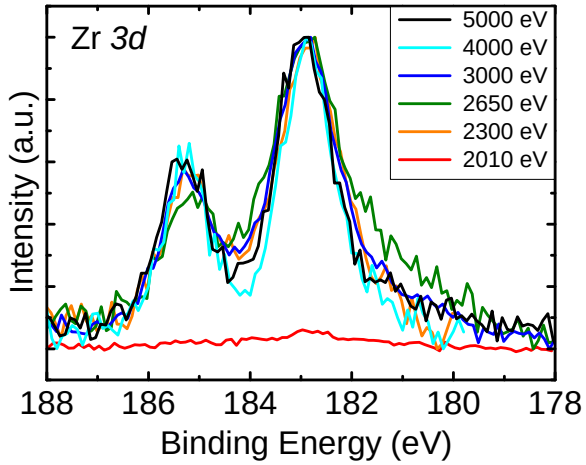

Fig. 2 HAXPES spectra of the Zr $3d$ core level of sample type (ii) discussed in the manuscript. Spectra normalized to the Zr $3d_{5/2}$ components, except for the $2010\,\mathrm{eV}$ spectrum which could not be normalized because the intensity is to weak.

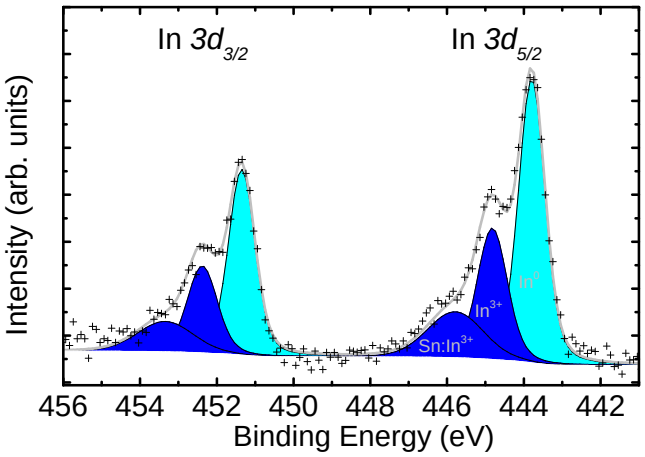

Fig. 4 HAXPES spectrum of the In $3d$ core level of sample type (iii). Spectrum recorded with a photon energy of $2010\,\mathrm{eV}$. In^{3+} components are shown in dark blue, In^{0} in light blue. Black crosses represent the experimental data, gray line is the superposition of all fit components.