

Wetting and dewetting of metals by sputter-deposited zirconia

P. Lackner^{1*}, J.-I. J. Choi^{1,2}, U. Diebold¹ and M. Schmid¹

¹ Institute of Applied Physics, TU Wien, Wien, Austria

² Institute of Basic Science, KAIST, Daejeon, Republic of Korea

Zirconia (ZrO_2) is a material commonly used as electrolyte in solid oxide fuel cells, in gas sensors or as high-k dielectric, but also as support for metal particles in catalysis. For metal particles supported by oxides, wetting effects can be a serious concern in applications. Under reducing reaction conditions, the oxides form thin films that encapsulate the metal particles. [1,2] This effect (known as strong metal-support interaction (SMSI) in the catalysis community) is usually limited to reducible oxides, where the ultra-thin wetting layer is formed by a substoichiometric oxide. However, zirconia, a material used in solid oxide fuel cells or as high-k dielectric, is considered non-reducible. Nevertheless, the same wetting and dewetting processes can be encountered, although the underlying process was until now unclear.

We have prepared few-layer-thick ZrO_2 films on Rh or Pt single crystals. ZrO_2 was deposited using a UHV-compatible home-built sputter source [3] (in 7×10^{-8} mbar O_2 and 8×10^{-6} mbar Ar), and then post-annealed in O_2 to form ZrO_2 islands. The sputter source can deposit Zr with high purity and very good reproducibility.

When the ZrO_2 films are annealed at high temperatures ($> 600^\circ\text{C}$) in 10^{-6} mbar oxygen, dewetting is encountered, i.e., oxide islands form and the bare metal surface gets uncovered in between. Annealing in ultrahigh vacuum instead leads to a structure akin to Stranski-Krastanov growth, i.e.,

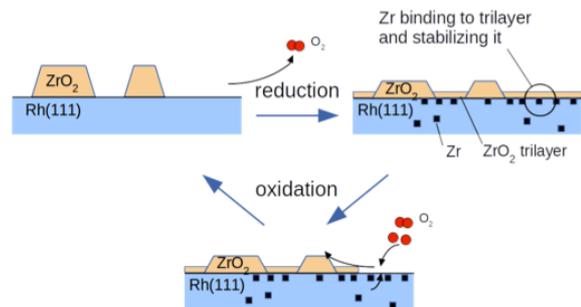


Fig. 1: Proposed mechanism of the SMSI effect for the non-reducible oxide ZrO_2 .

oxide islands with the metal in between covered by an ultra-thin oxide. XPS shows that the ZrO_2 trilayer is stoichiometric [4], as expected for a non-reducible oxide, thus the reason for the observed dewetting must be different from the usual variation of oxide stoichiometry. We propose a new mechanism for this wetting effect, which is alloying between Zr and the metal, modifying the metal-oxide bonding.

[1] S. J. Tauster et al., Science 211, 1121–1125 (1981).

[2] O. Dulub et al., Phys. Rev. Lett. 84, 3646 (2000).

[3] P. Lackner et al., submitted

[4] H. Li et al., J. Phys. Chem. C 119, 2462 (2015).

*Contact: lackner@iap.tuwien.ac.at