

Engineering of epitaxial oxide films for solar water splitting

H. Magnan^{a*}, D. Stanescu^a, A. Barbier^a, M. Rioult^a, A. Derj^a, E. Fonda^b, R. Belkhou^b, and F. Maccherozzi^c

- a. Université Paris-Saclay, CEA, CNRS, Service de l'Etat Condensé 91191 Gif sur Yvette Cedex, France
- b. Synchrotron SOLEIL, 91192 Gif sur Yvette Cedex, France
- c. Diamond light Source, harwell campus, didcot, OX11 ODE Oxfordshire, United Kingdom

* email : helene.magnan@cea.fr

The transformation of solar energy into chemical energy stored in the form of hydrogen, through photoelectrochemical water splitting is a promising method that has the important advantages of being environment friendly and free from carbon dioxide emission. Although, metal oxides are promising candidates for photoanode elaboration, their measured performances remain limited because of their low absorption coefficients and short hole diffusion lengths.

Fortunately, the photoelectrochemical properties of oxides can be improved by doping, by oxygen vacancies, by engineering the electronic or the crystallographic structure. In order to understand the physical mechanisms behind these improvements, we have studied the growth, crystal, and electronic structures of epitaxial oxide films (Fe_2O_3 , TiO_2) grown by atomic oxygen assisted molecular beam epitaxy. Such single crystalline samples are suitable model systems to study independently the effect of thickness, doping, and crystallographic structure effects on the photoelectrochemical properties. By using Extended X ray Absorption Fine Structure (EXAFS) and X-ray PhotoEmitted Electron Microscopy (X-PEEM), we have determined the role of crystallographic structure and surface morphology [1]. Our results demonstrate in the case of hematite the existence of an optimal oxygen vacancies concentration. In the case of TiO_2 , we show that rutile (100) is much more efficient than anatase (001) for solar water splitting [3]. Preliminary results about oxygen vacancies doping of these films will be also presented.

[1] M. Rioult et al., Surface Science 641, 310 (2015).

[2] M. Rioult et al. J. Phys Chem C 120, 7482 (2016)

[3] H. Magnan et al. J. Phys Chem C 123, 5240 (2019)

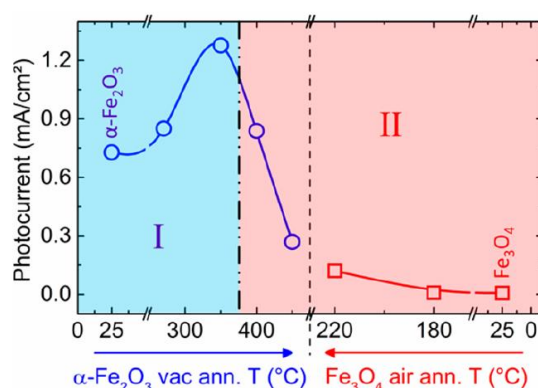


Figure 1 : Photocurrent as a function of annealing temperature of $\alpha\text{-Fe}_2\text{O}_3$ film (blue: annealing in vacuum), and Fe_3O_4 (red: in air annealing) from [2]