NAPLES, ITALY 23-27 JUNE
DSL2025 NAPLES
21st International Conference on Diffusion in Solids and Liquids

ABSTRACT

Model Single Crystalline Epitaxial Photoanodes for Solar Water Splitting

A. Barbier[1*], A Derj[1], M. Rioult[1], S. Datta[1], D. Stanescu[1], H. Magnan[1], J.-B. Moussy[1], C. Mocuta[2], M. Silly[2], R. Belkhou[2], P. Le Fèvre[2], J. Leroy[3], F. Maccherozzi[4]

[1] CEA/Saclay, Service de Physique de l'Etat Condensé, France;
[2] Synchrotron SOLEIL, France;
[3] IRAMIS/NIMBE Université Paris –Saclay, CEA, CNRS, France;
[4] Diamond Light Source, Oxfordshire, United Kingdom.

The development of environement friendly and sustainable chemical processes represents a major s ocietal challenge. The transformation of solar energy into chemical energy stored in the form of hydro gen, through photoelectrochemical water splitting is a seductive method that has the important adva ntages of being carbon dioxide emission free. Oxides / oxynitrides offer a very wide range of propertie s allowing for a multitude of applications including solar water splitting and/or CO2 reduction. Howe ver, their performance is often deceiving due to unfavorable band gap or charge recombination.

We have been developing model thin films for solar water splitting prepared by plasma-assisted mol ecular beam epitaxy for several years, in order to understand the relevant parameters to improve thei r performance. We studied the effectiveness of doping (Ti and O vacancies) in Fe_2O_3 [1,2], the role of electric polarization in $BaTiO_3$ [3, 4], charge carrier migration [5] and more recently the impact of nitro gen doping [6] where we used an original approach consisting in using the substrate as the oxygen su pplier during growth. The layers were characterized by a variety of laboratory and synchrotron radiatio n techniques. Each system allowed pinpointing the role of specific parameter in the improvement of t he photoelectrochemical activity of the film.

[1] M. Rioult et al., J. Phys. Chem C. 118, 3007 (2014),
[2] M. Rioult et al., J. Phys. Chem. C 2016, 120, 14, 7482–7490
[3] S. Datta et al., Thin Solid Films 607 (2016) 7-13
[4] M. Rioult et al., Appl. Phys. Lett. 107 (2015) 103901
[5] H. Magnan et al., The Journal of Physical Chemistry C (2020) 124 (19), 10315-10323
[6] A. Derj et al., Materials Advances, 2022, 3, 3135-3142