INSTITUT NÉEL Grenoble

Topic for Master 1 internship – Academic year 2019-2020

Title

Growth of TiO_2-Anatase catalyst films for water splitting

General Scope:

Titania is of interest among others for its photocatalytic behavior for hydrogen production from water splitting process. TiO_2 crystallizes in rutile and anatase phases. Rutile is the most thermodynamically stable structure at high temperature, whereas anatase, a natural-forming polymorph, is the most stable at room temperature, as well as the most photoactive. The best properties are obtained for the anatase-TiO_2(001) surface. This facet has the higher number of Ti active sites at the surface, all of them coordinated to five oxygen neighbors. However, the study of the (001) anatase is difficult because in natural crystals it covers less than 20 % of the surface. The other 80 % is covered by facets of the {101} family (Fig.1). One way to overcome this limitation is growing TiO_2 films with the desired face termination

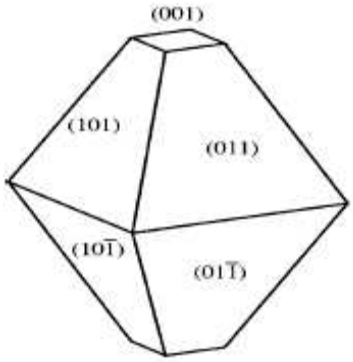

Fig. 1. Most stable Anatase crystal faces.

Research topic and facilities available:

TiO_2(001) films have already been grown by pulsed laser deposition technique (Fig.2). During the period of this internship the objective will be to growth high quality TiO_2(001) ultra-thin films by molecular beam epitaxy on STO(001) substrates and on BTO(001) films optimizing the conditions like e.g. substrate temperature and partial oxygen pressure.

The films will be prepared and studied *in-situ* using two interconnected chambers, the first one dedicated to MBE growth, the second one to the characterization by low energy electron diffraction (LEED), Auger electron spectroscopy and scanning tunnel microscopy (STM) techniques. During the internship the student will learn about these techniques and the fundamental of surface science.

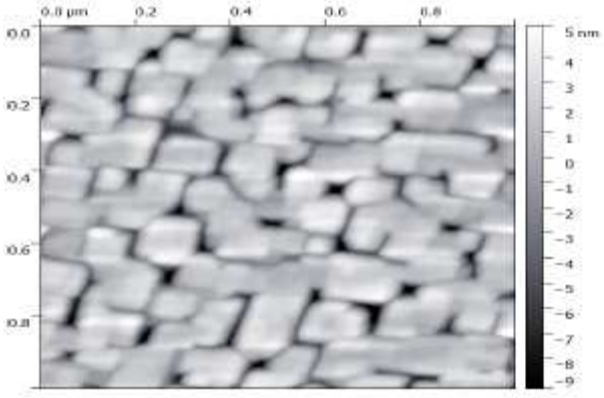

Fig. 2. AFM of TiO2-Anatase(001) / STO film. Thickness 40 nm.

Possible collaboration and networking:

This project is a collaboration with Xavier Torrelles from the Institute of Materials Science of Barcelona (ICMAB-CSIC)

Required skills: A good background in condensed matter physics, dexterity in experimental work.

Starting date: March 2020

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