NÉEL INSTITUTE Grenoble

Topic for Master 2 internship – Academic year 2023-2024

Title

Surface structure of TiO_2-Anatase (001) films by quantitative low energy electron diffraction

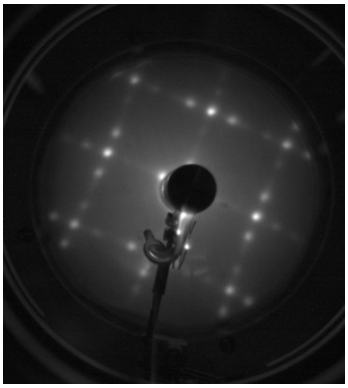
General Scope :

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. In the last years, we have grown (001) anatase in epitaxy on $SrTiO_3$(001) crystals by Pulsed Laser Deposition and by Molecular Beam Epitaxy (MBE) techniques (A. Crespo, *et al*. Applied Surface Science 632 (2023) 157586 10.1016/j.apsusc.2023.157586⟩. (001) anatase surface shows a (4x1) reconstruction and its photocatalytic properties depend on its detailed atomic structure.

Research topic and facilities available :

During the internship, epitaxial anatase (001) films will be grown by MBE following the two steps method described in the reference cited above, and the structure of its (4x1) reconstructed surface will by investigated by quantitative low energy electron diffraction (LEED). At least 2/3 of known surface structures have been determined by this technique. At this purpose, the intensity of several diffracted beams is measured as function of the incident electron beam energy in the region from 30 to 500 eV. It is then compared to the value calculated in the multiple scattering approximation theory for different trial structure models. These calculations will be performed using the viperLEED code, which is developed at the technological university of Vienna and will be implemented at the Néel institute.

An experimental set-up consisting of two interconnected chambers will be used. The first one is dedicated to MBE growth, the second one to the characterization by LEED, Auger electron spectroscopy and scanning tunnel microscopy (STM).



LEED of an anatase (001) film with (4x1) surface reconstruction.

Possible collaboration and networking :

This subject is developed in close collaboration with Xavier Torrelles from the Institute of Materials Science of Barcelona (ICMAB-CSIC). The LEED calculations will be performed in collaboration with the team from TU-Wien, which develops the viperLEED code.

Possible extension as a PhD : An extension as a PhD is possible, but it is not funded up to now.

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

Starting date : March 2024

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