LMGP/SIMAP **PHD THESIS OFFER 2021-2024**

Optimization of high performance nano-architectured electrode/electrolyte bilayers for reversible Solid Oxide Cells

Doctoral school / Starting date

IMEP2 / Starting date: 01/10/2021

Subject

CONTEXT

In the last decades, advanced thin film technology has enabled a wide range of technological breakthroughs that have transformed entire sectors such as electronics and lighting by the implementation of outstanding nanoscale phenomena in reliable products that involve ultralow contents of critical raw materials. In the future the energy storage sector could be revolutionized by the development of pocket-sized kW-range stacks based on **nano-architectured thin film reversible Solid Oxide Cells (TF-rSOCs)** that will be able, using gaseous fuel such as H_2, to efficiently store renewable electricity for applications where the use of batteries is inefficient due to size constraints or long term storage requirements, e.g. off-shore power generation or transportation. This requires the development of TF-rSOCs with low operating temperatures (around 500 ºC) and high efficiency to be able to store up to 100J/cm^3.

THESIS PROJECT

In order to be able to reach the very ambitious performance requirements for the TF-rSOCs at low operation temperatures (<500° C), in **this PhD thesis** we propose the **design, optimization and simulation of new electrode microstructures**. For this purpose **new deposition methodologies** will be used, using 2 chemical deposition techniques, i.e. Metal Organic Chemical Vapour deposition (MOCVD) and Atomic Layer Deposition (ALD) both individually and combined (at LMGP laboratory). In addition to the standard structural, chemical, morphological and electrochemical characterization, we will develop **simulation** (at SIMAP laboratory) in order to guide the design of novel electrodes. The influence of transport properties, oxygen reduction reaction (ORR) kinetics and architecture (multilayers and 3D) will be addressed by simulation.

OBJECTIVES

The main goals of the PhD thesis are:

1. **To develop novel electrode/electrolyte architectures with improved performance.**

   Several novel microstructures will be designed, such as: hierarchical microstructures with large catalytically active areas, interface-strained microstructures and grain boundary-rich microstructures. By combining defects (grain boundaries) and alternating dense and porous regions the functionality of the electrodes (ORR, ionic and electronic transport and current collection) will be locally optimized "per region" of the electrode.

2. **To understand and quantify the combined effects of architecture, enhance ionic conductivity and enhance ORR kinetics.**

   To assist the development of novel electrode/electrolyte half-cells, modeling will be used in order to explore various strategies based on architecture, enhanced ionic transport and enhanced ORR kinetics to optimize the design of electrodes. In addition, confrontation between simulation results and electrochemical measurement on half-cells will help us to gain a better fundamental understanding of the interplays between on one hand materials parameters (transport and ORR) and on the other hand architecture, grain boundaries and strain engineering of the films.

Scientific Environment

This project will be a collaboration between LMGP and SIMAP laboratories. The complementary experience will be combined in this project leading to a unique set of complementary competences for the student.

Within the **LMGP, Materials and Physical Engineering Laboratory**, the candidate will work in **the NanoMat team**, experts in chemical vapour deposition and functional oxide thin films. Within the **SIMAP, the PhD will work in the GPM2 team** at the forefront of material modelling and simulation. Located in the heart of an exceptional scientific environment, the LMGP and SIMAP offer the applicant a rewarding place to work.

This PhD thesis will be carried out in the framework of the European FET Proactive project "Harvestore" (http://www.harvestore.eu/) and of the Labex CEMAM dedicated to multifunctional architectured materials (https://cemam.grenoble-inp.fr/) The PhD student will have a strong interaction and the possibility of collaborating with the several groups within the European consortium, including the Catalonia Institute for Energy Research IREC (Spain), the Institute of Microelectronics of Barcelona IMB-CNM-CSIC (Spain) and Imperial College London (UK), among others.

LMGP Web Site: http://www.lmgp.grenoble-inp.fr/en

SIMAP Web Site: https://simap.grenoble-inp.fr/en

Profile & requested skills

The candidate must be graduated from an engineering school and/or with a Master 2R degree whose training focuses primarily on materials science, physics, chemistry or related field.

We are looking for a highly-motivated student with a strong interest in experimental physics and materials science. Interpersonal skills, dynamism, rigor and teamwork abilities will be appreciated. Candidates should be fluent in English and/or in French. In addition, well-written English will be highly appreciated.

Salary

Approximately 2100 €/month

Supervisors

Mónica BURRIEL (LMGP): monica.burriel@grenoble-inp.fr
David Jauffres (SIMAP): david.jauffres@simap.grenoble-inp.fr

LMGP: 3 Parvis Louis Néel, Grenoble INP, MINATEC, BP 257, 38 016 Grenoble cedex 1
SIMAP/GPM2: Batiment ECOMARCH, Domaine Universitaire, BP46, 38402 Saint Martin d'Heres cedex

Further information and Application

For further information don't hesitate to contact us.

To apply please send both supervisors by email **ASAP** and **before the 30th May 2020** your:

- Detailed Curriculum Vitae
- Cover letter explaining the motivation for the PhD work
- Transcript of marks obtained in Masters
- Contact details of two referees