2016-2017

Internship proposal (Master or final project engineering school) at LMGP Lab.

# Deposition of oxide thin films via Spatial Atomic Layer Deposition: Modelling approach for a process optimization

## Project description

In ever more challenging environmental conditions an increasing amount of scientific work is devoted to the investigation of new materials for energy applications. But apart from finding better materials, new processing tools need to be developed allowing the scalable deposition of high quality materials at low temperatures. Atomic Layer Deposition (ALD) is an attractive candidate since it has unique unrivalled features including: i) a highly precise control of layer thickness; ii) the capability of depositing uniform and conformal coatings even on high aspect ratio features; and iii) the possibility to deposit high quality films at low temperatures. These qualities are a result of ALD mechanism: ALD is a particular case of Chemical Vapor Deposition (CVD) in which the reaction is restricted to the sample surface, thus being self-limited. This is achieved by exposing the sample to the reactants at different time, i.e. in a sequence of pulses. In this way, the metal precursors are supplied and react with the surface, ideally forming a monolayer. Excess precursor is then purged, usually by evacuation. The second precursor is then injected and reacts with the chemisorbed layer forming a monolayer of the desired material plus by-products that have to be purged along with the excess precursor. The cycle is then repeated the necessary number of times to obtain a very precise film thickness. But also as a result of the ALD particular mechanism, deposition rates are very low and vacuum processing makes it complicated and expensive to scale up.

Recently, a new approach to atomic layer deposition (ALD) has been developed that doesn't require vacuum and is much faster than conventional ALD. This is achieved by separating the precursors in space rather than in time. This approach is most commonly called Spatial ALD (SALD). In the LMGP we have developing a novel atmospheric SALD system to fabricate active components for new generation solar cells and other applications, showing the potential of this novel technique for the fabrication of high quality materials that can be integrated into devices. Our system is based on an injection manifold head in which the different gas flows are distributed along parallel channels.

***References:*** *David Muñoz-Rojas*, and Judith L. MacManus-Driscoll. Materials Horizons, 1, 314-320, 2014.*

## Work requested (Subject internship)

The goal of this internship is to work within a team aiming at optimising the SALD system by using modelling approaches to optimize the injector head design. COMSOL will be used to evaluate the optimum head designs and the optimum deposition conditions for different head designs. The results obtained from the modelling will be use to fabricate improved head which will be tested in the system.

The LMGP has a long experience in modelling and houses state of the art experimental equipments for materials characterization.

## Location

Located in the heart of an exceptional scientific environment, the « Laboratoire des Matériaux et du Génie Physique » (LMGP) offers the applicant a rewarding place to work. The applicant will be integrated within a team and in close collaboration with surrounding laboratories (CEA-Grenoble, Institut Néel, SIMAP…).

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

## Profile & requested skills

We are looking for a highly motivated student who is interested to work in an inter-disciplinary group and on an interdisciplinary project. Experience in modelling with COMSOL or similar will be valued. Interpersonal skills, dynamism, rigor and teamwork abilities will be appreciated. Candidates can be fluent either in English or in French.

**Subject could be continued with a PhD thesis** : YES

**Allowance** : Internship allowance will be provided.

## CONTACT

David MUÑOZ-ROJAS: davidmunozrojas@gmail.com
Carmen JIMENEZ: carmen.jimenez@grenoble-inp.fr, Tel: 04 56 52 93 34
Daniel Bellet: Daniel.Bellet@grenoble-inp.fr