LMGP
Laboratoire des matériaux et du génie physique
une vision des matériaux

Grenoble INP

cnrs

UGA
Université Grenoble Alpes

2020-2021 Internship proposal at LMGP Lab.

Optimization of a Spatial Atomic Layer Deposition system by simulation

Abstract

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. We are also exploring alternative ways to control particle sintering and crystallization during film growth.

Project description

The goal of this internship is to work within a team aiming at optimizing 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. We use 3D printing to fabricate our optimized designs and test them in the SALD systems.
The LMGP has a long experience in modelling and houses state of the art experimental equipment for materials characterization. Simulation work in possible through remote access to the software at LMGP and thus the internship would be less affected by an eventual lab closure due to COVID19

Related Publications

Influence of the geometric parameters on the deposition mode in spatial atomic layer deposition: a novel approach to area-selective deposition

César Masse de la Huerta, Viet Huong Nguyen, Jean-Marc Dedulle, Daniel Bellet, Carmen Jiménez, **David Muñoz-Rojas***

Coatings, **2018**, 9(5), 5.

See also https://sites.google.com/site/workdmr/dmr/spatial-ald

Scientific environment:

The candidate will work within the LMGP, Materials and Physical Engineering Laboratory, in the Funsurf group

Located in the heart of an exceptional scientific environment, the LMGP offers the applicant a rewarding place to work.
LMGP Web Site: http://www.lmgp.grenoble-inp.fr/

Profile & requested skills:

The candidate must have a good ranking (top 25%) in master or engineering school. Ideally, (s)he should have some experience in surface chemistry and materials sciences. We are looking for a highly motivated student who is interested to work in an inter-disciplinary group and on an interdisciplinary project. Interpersonal skills, dynamism, rigor and teamwork abilities will be appreciated. Candidates should be fluent in English and have good writing and presentation skills.

Subject could be continued with a PhD thesis: YES provided there is funding

Allowance: Internship allowance will be provided

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