

## 2022-2023 Internship proposal at LMGP Lab.

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### Deposition of oxide thin films via Spatial Atomic Layer Deposition: in search of (new) high-quality oxide semiconductors for electronic and optoelectronic applications

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#### 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 deposition of high quality oxide films, ( $\text{Cu}_2\text{O}$ ,  $\text{ZnO}$ ,  $\text{TiO}_2$ ,...), by SALD. The final objective is to be able to tune the properties of the films both by adjusting the deposition parameters and via doping in order to use the materials in solar cells and TFTs, among others. The students will also participate in the development of new SALD processes to deposit new materials. This will be done in the framework of an International ANR project with Germany (with a group expert in the synthesis of new ALD precursors).

The physical properties (chemical composition, crystallographic structure, electrical conductivity, optical transparency, mechanical properties) of the films will be thoroughly investigated and optimized as well by using appropriate thermal annealing. The LMGP houses state of the art experimental equipment for investigating such properties. X-Ray diffraction (XRD), spectrophotometry, optical and electron microscopy will be routinely used to get a better understanding of the relationships between microstructure and physical properties for as-deposited and thermally treated films.

#### Related Publications

**Main publications from the team on the subject are:**

[Nature Communications volume 13, Article number: 5322 \(2022\)](#)

[Commun Mater 2, 78 \(2021\)](#)

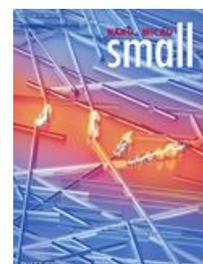
[ACS Applied Materials & Interfaces, 2021, 13\(18\), 21971–21978](#)

[Small, 2021, 17\(21\), 2007344](#)

[Chemical Engineering Journal, 2021, 403, 126234](#)

[Advanced Materials Technologies, 2020, 5 \(12\), 2000657.](#)

[Chemistry of Materials, 2020, 32, 12, 5153–5161](#)



See <https://sites.google.com/site/workdmr/dmr/spatial-ald> for a more comprehensive list

#### 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, in the framework of an international ANR project with Germany.**

**Allowance:** Internship allowance will be provided (~600 euros/mois)

**Duration :** 6 months

**CONTACT**

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