

## 2019-2020 Internship proposal at LMGP Lab.

### Atomic-level control over ultrathin 2D layers of Transition Metal Dichalcogenides obtained by a Molecular Layer Deposition route

### Synthèse de couches ultra minces de dichalcogénures de métaux de transition par dépôt moléculaires alternés en phase vapeur (ALD/MLD) et recuits.

#### **Abstract**

The main purpose of this research master internship is to implement an innovative fabrication of sulfide-based lamellar materials and ultimately 2D transition metal dichalcogenides (TMD), a recognized class of emerging materials. The student will achieve Atomic Layer Deposition/Molecular Layer Deposition of sulfide thiolates and the subsequent thermal treatment, in a dedicated reactor at LMGP, while monitoring the early stage of growth by ellipsometry. A specific equipment will be used to monitor the crystallization during annealing by Raman scattering. A great deal of the internship will be devoted to structural and chemical analysis of the 2D layer by various techniques.

#### **Project description**

2D-materials, especially transition metal dichalcogenides (TMD) [1], have recently received considerable attention since they are emerging as a class of exceptional semiconductor materials with many potential applications (supercapacitors, batteries, electronics and opto-electronics, flexible electronics, ...). However, a sizeable bottleneck for their full deployment stems from the lack of scalable fabrication methods with atomic scale precision. In the recent years, a 2-step Atomic Layer Deposition/Molecular Layer Deposition process and annealing has been used for the synthesis of 2D MoS<sub>2</sub> and WS<sub>2</sub> [2,3]. It has the advantage of being compatible with the manufacturing environment and avoid the use of toxic sulfur molecules as for instance H<sub>2</sub>S ("green" chemistry). However, as far as MoS<sub>2</sub> and WS<sub>2</sub> are concerned, the 2D crystallization is obtained by an annealing at a rather high temperature (> 800°C), which severely hinder the integration capabilities of those materials. Alternatively, Tin disulfide (SnS<sub>2</sub>), which is a semiconductor with a band gap in the range [2.2-2.35eV] (depending on the layer thickness), appears as a good candidate since it has a low melting point (865°C) in comparison to those of MoS<sub>2</sub> and WS<sub>2</sub>. Moreover, Tin is an earth-abundant metal with almost all of its oxide and sulfide derivatives (SnS, Sn<sub>2</sub>S<sub>3</sub>, SnS<sub>2</sub>, SnO et SnO<sub>2</sub>) being semiconductors and non-toxic.

The internship takes part of the collaborative ULTiMeD project, funded by the French ANR, which aims at **the atomic-level control over ultrathin 2D layers of Transition Metal Dichalcogenides by a Molecular Layer Deposition route**. The project mainly focusses on the investigation of the early stage of deposition and crystallization of 2D TMDs films processed with organosulfides (as Sulfur source alternative to H<sub>2</sub>S) in a custom-built portable reactor for Atomic Layer Deposition (ALD) [4-6].

Under the guidance of a post-doctoral fellow and PhD student, the successful Master candidate will prepare the ALD/MLD reactor at LMGP to receive the Tin precursor. He will achieve Atomic Layer Deposition/Molecular Layer Deposition of SnS<sub>2</sub> thiolates and the subsequent thermal treatment in the MOON reactor at LMGP. The growth will be monitored by ellipsometry (and possibly by residual gaz analysis). Some of the post ALD/MLD amorphous samples (thiolates) will be transferred to perform *in situ* Raman scattering measurements during thermal annealing at the LETI characterization platform. Post annealed samples will be checked by high resolution X-ray fluorescence (LETI), X-ray reflectivity, grazing incidence X-ray diffraction, X-ray photoelectron spectroscopy (CMTC, Grenoble INP) and Transmission Electron Microscopy (LMGP).

[1] Y.P. Venkata Subbaiah et al (2016), Adv. Funct. Mater **26**, 2046 ; [2] S. Cadot et al. (2017), Nanoscale **9**, 538 ; [3] S. Cadot et al. (2017), J. Vac. Sci. Technol. A **35**, 061502. [4] R. Boichot et al. (2016), J. Chem. Mater. **28**, 592. [5] M. H. Chu et al. (2016), Cryst. Growth Des. **16**, 5339. [6] E. V. Skopin et al. (2018), Nanoscale, **10**, 11585.

#### **Scientific environment:**

The master candidate will work within the LMGP (Materials Science and Physical Engineering), in team **NanoMat** in close collaboration with a post-doc, in the framework of the ULTiMeD project and with the other partners of the ULTiMeD project (C2P2, Lyon ; IPVF, Palaiseau, SOLEIL), as well as scientists at CEA Leti. Located in the heart of an exceptional scientific environment, the LMGP offers the applicant a rewarding place to work.

#### **Profile & requested skills:**

The candidate must be engaged in a research master program in physics, chemistry or material science or closely related science. She/he should also have ability and initiative to get to the heart of the problem and take it effectively through to completion; good interpersonal, communication and scientific presentational skills; good organizational and planning skills. Self motivation.

**Allowance:** Internship allowance will be provided

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