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

Grenoble INP

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2022-2023 Internship proposal at LMGP Lab.

Synthesis of Ga_xS chalcogenides by Atomic Layer Deposition/Molecular Layer Deposition

Abstract

The objective of this research internship is to synthesize metal Ga_xS chalcogenides. The student will achieve Atomic Layer Deposition/Molecular Layer Deposition (ALD/MLD) and thermal treatment of Ga-thiolates thin films in a dedicated reactor located in LMGP, while monitoring the process by *in situ* ellipsometry. Structural and chemical analysis of the thin films will be performed post deposition, by Raman scattering spectroscopy, X-ray photo-electron spectroscopy (XPS), X-ray fluorescence and Transmission Electron Microscopy. Specific equipment could be used to study the thiolate thin film crystallization by *in situ* X-ray diffraction. The internship student is likely to participate to a campaign of experiments at synchrotron SOLEIL (St Aubin) to study the thiolate deposition and annealing by *in situ* synchrotron X-ray techniques

Project description

2D-materials, especially metal dichalcogenides (MDs)[1,2], have received considerable attention recently since they are emerging as a class of exceptional materials with many potential applications. Beside the prototypical transition metal dichalcogenide (TMDs) MoS_2, WS_2, TiS_2, … there are several interesting lamellar MDs to investigate as precursors of new hybrid composites for emerging devices. The internship work will focus on **layered gallium sulfide (GaS) materials**. Gallium sulfide (**Ga_xS**) has two stable forms: **GaS and Ga_2S_3**[3]. Both forms are wide-band-gap semiconductors (Eg = 3.0 - 3.6 eV), making them promising candidates for optoelectronics and photovoltaics[4]. In particular, gallium sulfide thin films have been proposed as passivation layers in III-V semiconductors [5], anodes for Li-ion batteries[6] and buffer layers in CdTe solar cells[7]. Atomic Layer Deposition , as well as Molecular Layer Deposition, are based on sequential, self-limiting surface reactions that allow conformal film growth with precise thickness control. They are ideal techniques for depositing scalable ultrathin inorganic and organic films. Indeed, we develop a 2-step process[8] which consists in depositing a metal-thiolate thin film by ALD/MLD on wafers, then, the metal-thiolate, which was formed after the reaction of the metal precursor and organic sulfide molecule (1,2-ethanedithiol), is transformed into the target material by annealing in a controlled atmosphere[8,9]. This approach aims to find alternatives to the very toxic H_2S molecule currently used for the growth of 2D MDs by ALD/MLD and to improve the control on the thin film crystallization and texture.

The successful Master candidate will achieve ALD/MLD of Ga-thiolates thin films in a dedicated reactor in LMGP, on thermal SiO_2 and other substrates, while monitoring the growth by *in situ* ellipsometry (and possibly by residual gaz analysis). Post ALD/MLD thiolate thin films could be transferred into specific equipment to perform *in situ* Raman scattering measurements at the LETI characterization platform or *in situ* XRD at Grenoble-INP characterization platform (CMTC), to study the crystallization during the thermal treatment. Post annealed samples will be checked by high resolution X-ray fluorescence, X-ray reflectivity, in-plane X-ray diffraction, X-ray photoelectron spectroscopy (CEA-Leti) and Transmission Electron Microscopy (LMGP). The internship student is likely to participate to a campaign of experiments at the synchrotron SOLEIL (St Aubin) to be carried out by June 2023.

This internship work takes part of the collaborative ULTiMeD project, funded by the French ANR, which aims at the atomic-level control over ultrathin layers of lamellar metal dichalcogenides by a Molecular Layer Deposition route. The project mainly focusses on the investigation of the early stage of deposition and crystallization of lamellar metal dichalcogenide ultra-thin films processed with organosulfides (as a sulfur source alternative to H_2S) in a custom-built portable reactor for Atomic Layer Deposition (ALD) [10-12].

[1] Y. P. Venkata Subbaiah et *al.* (**2016)** Adv. Funct. Mater. 26, 2046 ; [2] W. Hao et *al*. (2019) 2D Mater. **6** 012001 ; [3] R. M. A. Lieth *et al* 1966 *J. Electrochem. Soc.* **113** 798 **;** [4] X. Meng et *al*. (2014) Adv. Funct. Mater. 24, 5435 ; [5] X. Cao, *JVST. B* **1998**, 2656 ; [6] X. Meng et al. *Adv. Funct. Mater.* **2014,** 5435 ; [7] E. Cuculescu et al. *J. Optoelectron. Adv. Mater.* **2006**, 1077 ; [8] S. Cadot et *al*. *Nanoscale* **2017**, 538 & S. Cadot et al. *JVST. A* **2017**, *35*, 061502 ; [9] P. Abi Younes et *al*. (2022) To be published ; [10] E. V. Skopin et *al*. *Nanoscale* **2018**, 11585 ; [11] R. Boichot et *al*. **2016**, DOI 10.1021/acs.chemmater.5b04223; [12] M. H. Chu et *al*. *Cryst. Growth Des.* **2016**, 5339.

Scientific environment:

The master candidate will work within the LMGP (Materials Science and Physical Engineering), in team **NanoMAT**, in the framework of the ANR ULTiMeD project. He will interact on a regular basis with scientists from IPVF (N. Schneider) and CEA Leti (N. Gauthier). 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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