Tool Development for spatial thickness and composition distribution prediction in combinatorial PLD thin films

Supervisors

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Number of Candidates

3

Backgrounds of Candidates

Candidate 1: The candidate preferentially has an interest in materials properties, with some laboratory experience. An interest in synthesis methods, such as solid-state synthesis or sol-gel synthesis is advantageous. Experiences with synthesis, XRD, PLD, and SEM are desirable.

Candidate 2: The candidate preferentially has an interest in materials properties, with some laboratory experience. Cleanroom experience is advantageous. Experiences with XRD, PLD, and SEM are desirable.

Candidate 3: The candidate preferentially has an interest to programming, with some python experience. An interest in tackling combinatorial materials science by programming is advantageous.

Project Descriptions

Thin films are widely used in research of functional layers and renewable energy devices. Combinatorial pulsed laser deposition (cPLD) co-deposits at least two source materials onto a substrate to create a thin film with a compositional gradient. This film presents a continuous composition spread library of the materials used during the deposition and contains any stoichiometry between the two source materials. The spatial distribution of composition and thickness of such thin films can be predicted by, e.g., pyPLD [1], a python package, only requiring the specific growth rates of source materials and geometry of the PLD system as input. To help implementing such a tool at UiO, we offer three different summer projects connected as shown in fig. 1.

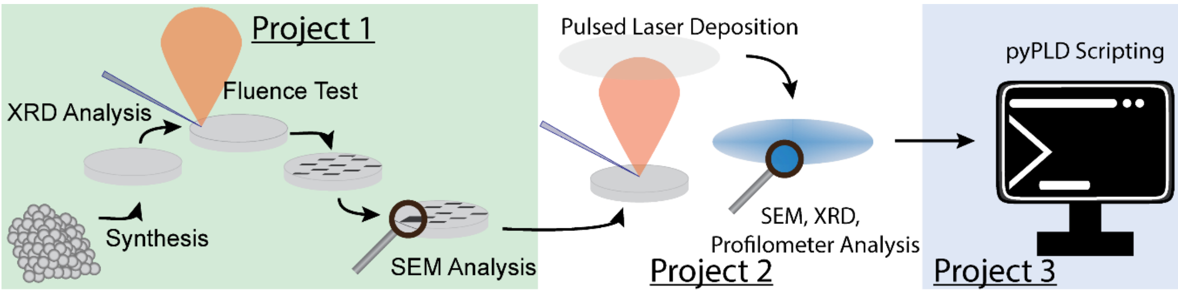

Figure 1: The three projects and their connections outlined. A final step involving all three parts is to determine the validity of the model by synthesizing a combinatorial thin film.

Project 1: In this project, the student will synthesize pellets for PLD deposition, and investigate systematically the influence of laser fluence on properties (surface morphology, changes in composition) of the pellet itself. The student will be introduced to different manufacturing methods of pellets (i.e., pellet pressing, sintering in different atmospheres, etc.), characterize the pellets by XRD and SEM, and finally investigate the ablation craters induced by the laser during the fluence test. Depending on the student's ability, the fluence tests can be carried out by the student or by the supervisors with the student present. Segmented PLD targets will be synthesized in discussion with project 3.

Project 2: In this project, the student will investigate the thickness of thin films deposited on wafers by Profilometer, SEM, and XRD. The goal is to determine the material-specific growth rates and parameters, needed as iput for pyPLD, by depositing and characterizing binary thin films. The pellets will be provided by the supervisors or project 1, and the characterization process will be coordinated with the needs of project 3. In the end, a library of experimental data will be obtained. Finally, combinatorial thin films will be made to test the predictions of project 3.

Project 3: In this project, the implementation of pyPLD in a structured and simple manner at UiO is in focus. The goal is to develop a code and tweak its settings (mostly geometric parameters) such that the program reflects the PLD located in the MiNaLab. Additionally, an easy way to incorporate experimental data from project 2 will be developed. Finally, the database of material-specific binary growth rates will be used to predict spatial distributions of i) composition and ii) thickness of combinatorial thin films.

[1] Lysne, Hogne, et al. "Improved methods for design of PLD and combinatorial PLD films." *Journal of Applied Physics* 132.12 (2022).