Molecular dynamics study of the initial stages of thin film growth under energetic conditions

Internship duration: 5 months Starting period: 15 March 2020

Remuneration: 590€/month Financial support: ANR INTEGRAL Project

Supervisors: MASTAIL Cédric, PIZZAGALLI Laurent

Context:

Nanoscale metallic thin films have been used for many decades for various technological applications, including microelectronics, optoelectronics or functional overlayers to modify/improve the properties of structural materials, as well as their reliability. Over the years, many studies have demonstrated **a complex dependence** of film microstructure and resulting properties on the deposition conditions[1] (*i.e.* kinetic energy of deposited particles, nature and temperature of substrate) and on their characteristics[2] (surface mobility, chemical reactivity). Understanding initial growth stages and their influence on the evolution of film microstructure (grain size and texture) and properties (stress state, defect density, mechanical attributes) is the main objective of the **INTEGRAL** project funded by the ANR. A central part of this project will be the implementation of a robust and reliable **multiscale computational modelling** of thin film growth over realistic time scales to address issues of polycrystalline thin film growth and **stress** generation and relaxation processes.

Master 2 internship:

Upstream in this project, this M2 internship aims to investigate, by **molecular dynamics (MD)**, the early stages of growth under energetic conditions. As experimental observations point to different growth modes, 3D vs 2D respectively [1], the cases regarding high mobility - Cu/Si - and low mobility - Mo/Si - metals will be studied. The role of the kinetic energy of the incoming particles on the interfacial structure, growth mode and surface morphology as well as defect formation and migration, will be explored.

The first part of the internship will consist in a validation of existing interatomic potentials (Cu-Si and Mo-Si) at high-deposited energy (~ 200 eV) and elevated temperature (~600K).

In a second part, these potentials will be used in MD simulations of defect formation and diffusion as well as to study the chemical reactivity at the metal/silicon interface to gain insight in the mechanisms of silicide formation.

Continuation to PhD:

The work could be extended in the frame of a Ph.D. thesis. The applicant will actively participate to the development of a code based on kinetic Monte Carlo approach as well as experiments to achieve the objective of the INTEGRAL project. The developed code will incorporate elementary mechanisms at the atomistic level (adsorption and diffusion) and the corresponding energy barrier heights, identified using both MD and ab initio DFT calculations so as to depict realistic growth of metallic thin film on silicon substrate under energetic conditions.

The outcome of the code (example of kMC simulation for homo epitaxy of Cu given in fig1) will be benchmarked against dedicated **experimental studies** (structural, electrical and optical layer properties) thanks to ***in situ*** and **real-time** diagnostics available in the laboratory.

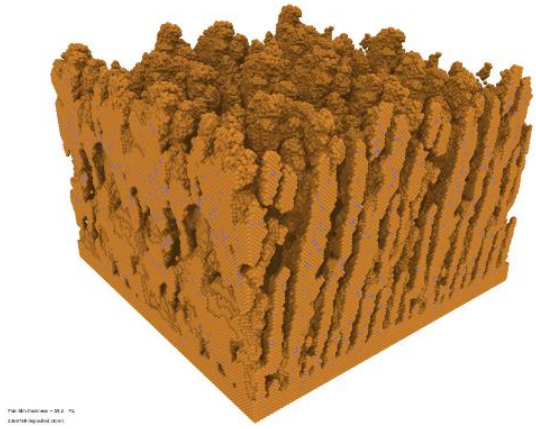

fig1; kMC simulation of homo epitaxy of Cu

Keywords: Thin Film Growth, Molecular Dynamics simulations (MD), Interface reactivity

Candidate profile

Highly motivated candidates in master degree or equivalent with a background in materials science and / or physics. Previous knowledge in molecular dynamic simulation or any other field that could benefit the project would be appreciated.

Application procedure

For additional information about the project and/or the recruitment process, please contact MASTAIL Cédric (cedric.mastail@univ-poitiers.fr, Tel: +33 (0)5 49 49 67 38)

The candidate should include a CV, a cover letter and at least one recommendation letter. The deadline for application is **8 February2019**.

1 B. Bouaouina, C.Mastail, *et all* , "*Nanocolumnar TiN thin film growth by oblique angle sputter-deposition: Experiments vs. simulations*", Materials & Design 160, 338 (2018) / G. Abadias, E. Chason, *et all*, "*Review Article: Stress in thin films and coatings: Current status, challenges, and prospects*", Journal of Vacuum Science & Technology A 36, 020801 (2018)
2 G. Abadias, *et all*, *"Real-time stress evolution during early growth stages of sputter-deposited metal films: Influence of adatom mobility"*, Vacuum 100, 36 (2014).

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