Ph.D proposal

Institut Pprime, Poitiers (FR)

Multi-scale computational study of the dependence between thin film properties and deposition parameters during energetic sputter deposition process

Internship duration: 36 months

Starting period: **immediately available and no later than October 15, 2021**

Remuneration: 1500€/month

Financial support: ANR INTEGRAL Project

Supervisors: Grégory ABADIAS and Cédric MASTAIL

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.

PhD tasks and objectives:

The primary aim of this Ph.D. thesis is to gain understanding on the influence of the deposition parameters on the initial thin film growth stages via the development of a realistic-growth-conditions code based on kinetic Monte Carlo (kMC) approach. To simulate the growth of metallic thin films on silicon substrate under energetic conditions as realistic as possible, the developed code will incorporate relevant elementary mechanisms determined at the atomistic level. In this aim, the candidate will first perform calculations using advanced ab-initio program package (VASP) and Molecular Dynamic software package (LAMMPS).

The candidate will then **determine driving mechanisms which occur during the growth:** i) potential energy surface ii) favourable adsorption configurations as well as adatom diffusion anisotropy, iii) surface/subsurface mechanisms (desorption, dimer formation and diffusion, nucleation, attachment and detachment to an island, etc.) depending on crystallographic orientation. Specific mechanisms resulting from the energy deposited by impinging particles, such as **defect creation** and relaxation processes, enhanced diffusion, re-sputtering, will be addressed by attributing an initial velocity to the incoming particles during MD simulations. The relevant mechanisms will then be implemented to upgrade an existing single-lattice kMC code, to mimic homo-epitaxial systems during sputter deposition process.

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The next step will be to investigate the influence of **atomic mobility** by focusing on Cu/Si and Mo/Si systems, as representative of low and high melting point (Tm) metals, respectively. A detailed and consistent picture of **interfacial reactivity** during the deposition based on both numerical (DFT, MD) and experimental approaches will be realised. Identified mechanisms at the metal/silicon interface will then be implemented in the kMC code to study their influence on diffusion, nucleation, and thin film growth, as representative of hetero-epitaxial systems.
To complete this multiscale methodology, the outcome of the code will be benchmarked against dedicated **experimental studies** thanks to ***in situ*** and **real-time** diagnostics available in the laboratory, to which the candidate could actively participate. The microstructure evolution during the first growth stages will be monitored by coupling surface differential reflectance spectroscopy (SDRS), electrical resistivity and MOSS stress measurements. In addition, phase transitions or silicide formation will be monitored using *in situ,* synchrotron-based, XRD techniques.

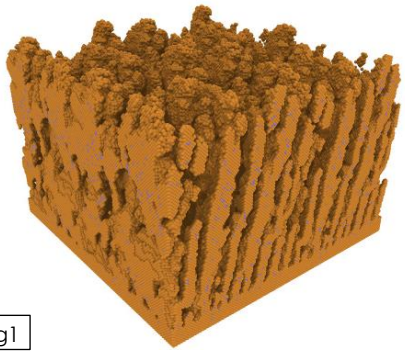

Fig1

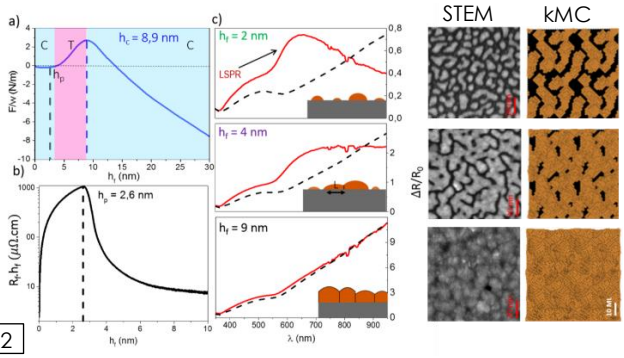

Fig2

Example (Fig1) of Cu growth morphology predicted by kMC simulation (Fig2) complementary kMC, STEM and in situ real-time diagnostics (stress a), resistivity b), reflectivity c)) analysis of initial stages of Cu sputter deposited layers.

Keywords: Thin Film Growth, kinetic Monte Carlo (kMC), Molecular Dynamics (MD), density functional theory (DFT), interface reactivity, multi scale approach

Candidate profile

Highly motivated candidates with a **Master degree** (or equivalent) in condensed matter physics or materials science and prior experience with computer simulations. The candidate should have some skills in programming languages (Fortran, C ,Python, etc), Linux. Basic knowledge in parallel computing will be appreciated.

Application procedure

Applications, including a CV, Master 1 and 2 marks, a cover letter and at least one recommendation letter, should be sent to Cédric Mastail (**cedric.mastail@univ-poitiers.fr**, Tel: +33 (0)5 49 49 67 38) and Grégory Abadias (**Gregory.Abadias@univ-poitiers.fr**, Tel: +33 (0)5 49 49 67 48)

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