Post-Doctoral position

Institut Pprime, Poitiers (FR)

Multi-scale computational modelling of polycrystalline thin film growth during energetic sputter deposition process and study of the dependence between stress generation and deposition parameters

Duration: 20 months

Starting period: 1 December 2020

Remuneration: between 2648.79 € and 3768.24 € / month according to experience, before deduction of taxes.

Financial support: ANR INTEGRAL Project

Supervisors: Grégory ABADIAS and Cédric MASTAIL

Keywords: kinetic Monte Carlo (kMC), K-Art, Stress, Multi-Scale approach, Grain Boundary, Polycrystalline thin Film Growth

Context:

Nanoscale thin films have been used for many decades for various technological applications, including microelectronics, optoelectronics, as well as protective or functional overlayers to modify/improve the properties of structural materials. Nowadays, research in the field remains exceptionally active as new emerging fields related to plasmonics or energy-harvesting applications rely on the synthesis of nanoparticles/nanowires with controlled shape and size distributions or involve a 3D integration of nanoscale layers into complex architectures for the next generation of electronic devices, to cite a few.
If deposition processes, based on either Chemical (CVD) or Physical Vapor Deposition (PVD) techniques, are routinely employed, the interdependence of many deposition process parameters, renders the task of controlling the growth process challenging, and in most cases results to an empirical tuning of these parameters. 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). This is illustrated in some of our recent works on Cu-Ge alloy thin films[3] and glancing angle deposition (GLAD) of TiN films[4].
Therefore, the need for a deterministic approach leading to a better understanding of the elementary growth processes is highly desirable. Computational modelling based on **numerical simulation** offers a comprehensive approach to fulfil this goal and contributes to provide a predictive and reliable tool towards end-users. To simulate the full growth process, from condensation of the vapor flux to the nucleation stage and towards the formation of thicker layers, over a realistic time scale comparable (order of seconds or minutes) with the experiments, requires a **multi-scale modelling.** 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.
The aim of the INTEGRAL project is to implement a robust and reliable multiscale computational modelling of thin film growth over realistic time scales with the ultimate goal to address **stress generation and relaxation** processes into a single, multi-methods simulation package. This computational-driven approach is based on a **kinetic Monte Carlo (kMC)** scheme, which will encompass both on-lattice and off-lattice models to address all interdependent issues of defect creation, chemical intermixing and **grain boundaries (GB) formation/migration during polycrystalline** film growth. Specifically, the project will address fundamental aspects of the growth process of

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polycrystalline thin films with emphasis laid on the **GB formation/evolution**, **surface faceting**, **stress relaxation** and the **defect creation/evolution** related to energetic deposition process, as also the early growth stages such as **interfacial reaction**, **nucleation and growth**.

Objectives and tasks of the post-doc fellowship:

The first objective is to extend the current kMC code developed by the group (and based on a single rigid lattice, see Fig. 1) to the case of **polycrystalline** thin film growth in order to account for the issue of GB formation and grain misorientation. To this aim, the post-doc fellow will implement a **multiple-network** scheme in the kMC code (mn-kMC), e.g. by using several rigid networks following Huang's[5] approach.
Particular emphasis will be placed on the dynamics of GB formation and the role of energetic species on metal and/or silicon diffusion. Also, defect annihilation at the free surface and at the GB will be implemented leading to thin film relaxation. This will give a comprehensive picture of the microstructural changes of polycrystalline films, and will allow for the identification of the origin of the structural and morphological evolution.
Beyond this, the final objective is to address the origin and evolution of intrinsic stress during thin film growth using **off-lattice** kMC. Therefore, the second part of the work will be dedicated to investigate at atomic scale, the crucial role of GBs on the **dynamic stress evolution** (generation and/or relaxation) during growth by means of a comprehensive description of the diffusion mechanisms near GBs (see Fig. 3). One suitable approach is the combination of the developed mn-kMC code with **kinetic Activation-Relaxation Technique** (k-ART)[6] code, which is an off-lattice, self-learning, on-the-fly identification and evaluation of activation barriers. The fulfilment of this objective requires an acquaintance to the inner works of the k-ART software: to this end a research stay is planned in the group of Pr. Mousseau (Montreal, Canada) who developed this software.

The outcome will be benchmarked against experimental validations (structural, electrical and optical layer properties) thanks to the unique palette of in situ and real-time diagnostics available at Pprime Institute (see Fig. 2).

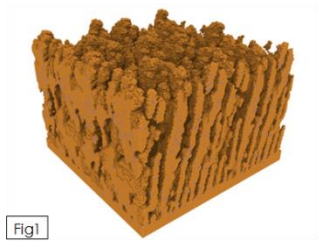
Fig1

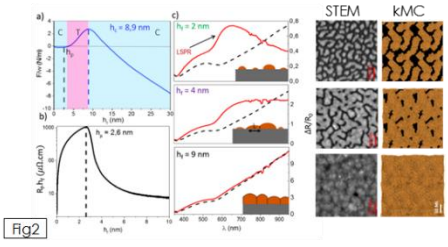

Fig2

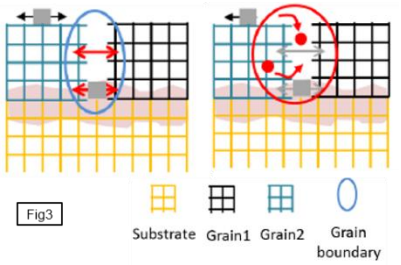

Fig3

Example of Cu growth morphology predicted by kMC simulation (Fig1), complementary kMC, STEM and in situ real-time diagnostics [stress a), resistivity b), reflectivity c)] of initial stages of sputter deposited Cu layers (Fig2) Schematic diagram showing elementary processes (surface diffusion, defect creation, interdiffusion, GB formation and incorporation of excess atoms at the GB (Fig3).

Candidate profile

Highly motivated candidates holding a **PhD degree** in condensed matter physics or materials science and competences in computer simulations. Prior experience in the field of surface science or thin film growth would be appreciated.

The candidate should have good **skills in programming languages** (Fortran, C, Python, etc), Linux. Basic knowledge in parallel computing will be appreciated.

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Application procedure

Applications, including a CV, a cover letter and two recommendation letters, 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)

The deadline for application is **1st October 2020**.

References

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