Master 2 internship subject

Academic year 2023-24

A numerical study of pattern formation in Cu ultrathin layers

Supervisors	Cédric MASTAIL	Grégory ABADIAS	Anny MICHEL
Internship funding	ANR INTEGRAL	Duration	5/6 months
Remuneration:	591.51€ corresponding to 151.67h/month		
Continuation in thesis?	**Yes**		
Thesis funding	Ministry scholarship		

Context and description of research project

Nanoscale metallic thin films have been used for many years in technological applications, such as microelectronics, optoelectronics for instance. Over the years, numerous studies have demonstrated a complex dependence of the film microstructure and the resulting properties on the deposition conditions (i.e. deposition rate, substrate temperature, kinetic energy of the deposited particles) and reactivity with the substrate. In this respect, the nature of the interfaces (chemistry, structure, spatial extent and roughness) is anticipated to strongly affect the subsequent film growth[1].

Understanding the initial growth stages and their influence on the evolution of film microstructure (grain size and texture) and properties (stress state, defect density, mechanical properties) was the main objective of the **INTEGRAL project** funded by the ANR.

The central part of this project concerned the development of a code based on a kinetic Monte Carlo (kMC) algorithm that allows to reproduce the homoepitaxial growth of Cu/Cu(001) by considering the angular and energy distribution of the deposited species, which are the main specificities of the sputter deposition process. One key finding is the development of a self-organized nano-structuration of Cu layers with a pattern formation that depends on deposition conditions (substrate temperature, angle of incidence), in good agreement with the literature results of Raberring et al. [2] (see figure 1 below).

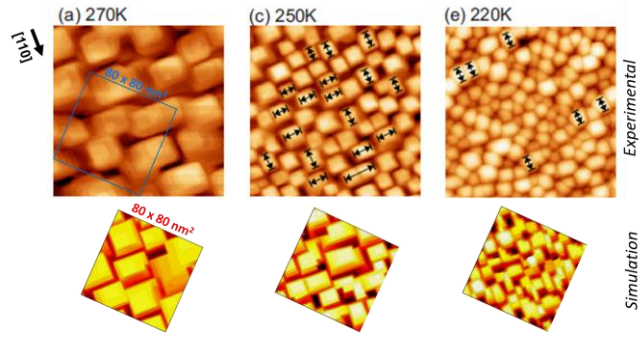

Figure 1: Literature results (top) of Raberring *et al.* of self-organized nano-structuration of Cu layers obtained for an incident angle of 85° at different temperatures[2], and our kMC simulated results obtained for the same conditions.

[1] B. Krause, G. Abadias et al., "Interfacial Silicide Formation and Stress Evolution during Sputter Deposition of Ultrathin Pd Layers on a-Si » ACS Appl. Mater. Interfaces 11, 39315 (2019)

2 F.L. W. Raberring et al. , "*Oblique incidence deposition of Cu/Cu(001): Enhanced roughness and ripple formation"*, PHYSICAL REVIEW B 81, 115425 (2010)

The aim of this M2 internship, connected to the INTEGRAL project, is to gain further understanding on the origin of the nano structuration mechanisms. To this end, a systematic numerical study will be employed using the developed kMC code.
As a first step, the candidate will investigate the **influence of the deposition parameters** on the characteristic features of Cu nano-structures (period, height, aspect ratio, etc…). *In a second step*, the growth of Cu layers on **pre-patterned substrates** (ripples) will be explored under different incidence angle conditions. The evolution of the film morphology from initial stages up to the formation of a continuous layer will be investigated. The morphological attributes (column shape, porosity, etc…) will be examined and discussed based on literature results.
This work will be continued during a PhD thesis on the broader subject of initial growth stages of thin films deposited by magnetron sputtering. It will be based on the combined use of numerical simulations and experimental work. Two following issues will be addressed: i) the impact of energetic species on film microstructure and defect formation, ii) the influence of growth interrupts on island density and morphological transition thicknesses (percolation and continuity), and iii) the influence of interface reactivity on the growth mode.
In the latter case the candidate will use the recently developed version of the kMC code to simulate hetero-epitaxial growth (e.g., Cu on Si). He/She will participate to the update the code to implement kinetic Activation-Relaxation Technique (k-ART)[3] scheme, which is an off-lattice, self-learning, on-the-fly identification and evaluation of activation barriers. The fulfilment of this objective will be facilitated thanks to close collaboration with the developer of the k-ART code, Pr. N. Mousseau (University of Montreal, Canada).

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 pursuing a master degree (or equivalent) in materials science and / or physics are encouraged to apply. Previous knowledge or experience in programming or any other field that could benefit the project would be appreciated.

Contacts:

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Application procedure

The candidate should include a CV, a cover letter and at least one recommendation letter. The deadline for application is 5 February2019.

[3] F. El-Mellouhi, N. Mousseau, L. J. Lewis, "*Kinetic activation-relaxation technique: An off-lattice self-learning kinetic Monte Carlo algorithm*", Physical Review B 78, 153202 (2008). / 0scar A. Restrepo, N. Mousseau, F. El-Mellouhi, O. Bouhali, M. Trochet, C. S. Becquart, "*Diffusion properties of Fe–C systems studied by using kinetic activation–relaxation technique*", Computational Materials Science 112, Part A, 96 (2016). / G. K. N'Tsouaglo, L. K. Béland, J. - F. Joly, P. Brommer, N. Mousseau, P. Pochet, "*Probing potential energy surface exploration strategies for complex systems*", Journal of Chemical Theory and Computation 11, 1970 (2015).