'Physique et Chimie des Matériaux' – ED 397 – année 2022

PhD project for funding, to send by 28/02/2022 to

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Research unit (full name + acronym) : Institut des Nanosciences de Paris INSP

Team if applicable : Physico-chimie et dynamique des surfaces

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Nber of phD under supervision 0 Participation to supervisor training? no Year

Co-supervisor : HDR? select Position : select

Tel email :

Research unit :

International co-supervision ? select

Keyword 1 : kinetic Monte-Carlo simulation Keyword 2 : 2D materials

Keyword 3 : epitaxy Keyword 4 : Fokker-Planck equation

Select co-funding programme if applicable : select

Project title : Theoretical investigation of the growth of 2D silicene and germanene

Project Description :

2D-materials are promising candidates for both fundamental science and electronic and photonic applications. After the development of graphene, a significant interest is devoted to silicene and germanene due to their exotic properties, band-gap and easy integration in devices. The production of these 2D layers by molecular beam epitaxy is under extensive investigation to improve the quality and sizes of the flakes produced in experiments. The need for a better control of the growth procedures is clear and requires understanding of the growth mechanisms. Different substrates have been explored to host these layers, from metals to hBN, graphene, transition metal dicalcogenides etc. In particular, dedicated experiments have been performed at INSP for the growth of Si and Ge on metallic substrates revealing the importance of alloying [1]. However, the way to control the morphologies and properties of the resulting layers remains unknown. It requires new modelization tools and a strong coupling between theory and experiments.

The best numerical tool to investigate the growth dynamics is kinetic Monte-Carlo simulations (KMC) [2]. Thanks to a number of controlled approximations, they can efficiently describe the dynamics of realistic multiscale models : they can account for atomistic scales and describe self-organization up to micrometer scales, and include atomistic events and describe growth up to experimental time scales [3]. These simulations have recently been successfully implemented to describe the growth of silicene on graphene. They revealed a new 2D growth mode under dewetting conditions [4]. This new mode leads to the growth of large silicene flakes under certain conditions, and allows to rationalize experiments carried out on these systems, Fig. 1.

The goal of this thesis is twofold. First, we will develop a KMC framework for the simulation of the growth of silicene and germanene layers on different substrates, Ag(111), Al(110) etc, that are investigated experimentally at INSP. We will use a rejection-free KMC code of a on-lattice model that will include the atomic deposition, diffusion and attachment/detachment processes. They will be made dependent on different configurations (local height, local configuration etc) to account for different effects (van der Waals interactions, local stoichiometry etc). We will account for different parameters such as crystalline anisotropies and mobilities by varying the diffusion barriers and geometries of the lattices. Of special interest will be the description of alloying that was revealed on Ag substrates at INSP in some temperature range, and that might be detrimental. To this end, we will include a two species model with extra possible atomic processes, especially intermixing. In this case, the model describes both the film height and a local composition (film or substrate atoms) that are free variables subject to the Monte-Carlo procedure. We will also investigate the influence of the film/substrate interactions, first the weak Van-der-Waals interactions that allow the 2D growth, but also long-range elastic interactions. The latter may occur in lattice-mismatched coherent conditions, but also when buckling occurs, and may enforce strain in the overlayer and Moiré patterns. The simulations will be parametrized both with the ab-initio calculations for the diffusion energy barrier and atomic bonding, and experimental statistical properties. They will be finely tuned with back-and-forth comparison with experiments to rationalize growth mechanisms. A systematic analysis of the modelization will be done in order to shed some new light on the different possible growth modes. In a second step, we will derive a theoretical coarse-grained description of this dynamical problem thanks to a Fokker-Planck description dedicated to 2D epitaxial growth. This theoretical framework will enable to describe large scale statistical properties and will be based on the simulation and experimental outcomes. Overall, this work is expected to reveal new fundamental growth mechanisms that rule the crystal growth of 2D materials, but also procedures that will guide experiments for the production of new materials.

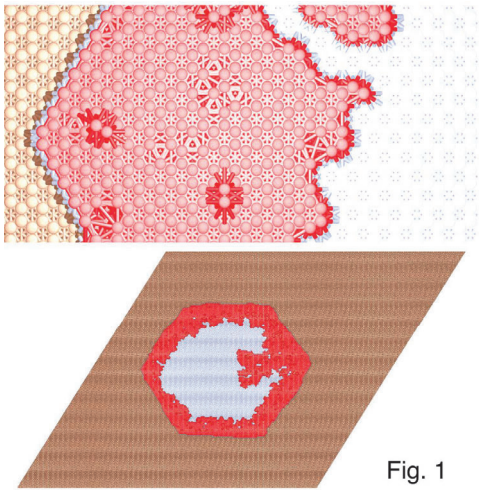

Fig. 1

References

[1] Curcella A., Bernard R., Borensztein Y., Lazzeri M., Resta A., Garreau Y., Prévot G., 2D Materials 4 (2017) 025067
[2] Curcella A., Bernard R., Borensztein Y., Pandolfi S., Prévot G., Bellstein J. Nanotechnol. 9 (2018) 48
[3] Gaillard P., Aqua J.-N., Frisch, T., Physical Review B 87 (2013) 125310
[4] Ben Jabra Z., Aqua J.-N. et al, ACS Nano 2022 (to be published)