Master 2: ***International Centre for Fundamental Physics***

INTERNSHIP PROPOSAL

Laboratory name: INSP
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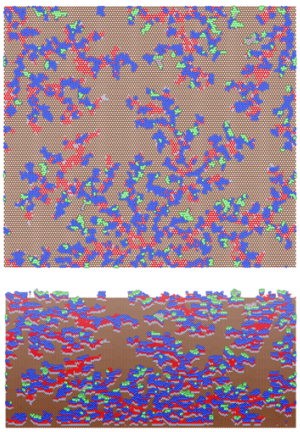
Internship location: INSP Jussieu 22-12
Thesis possibility after internship: YES
Funding: YES If YES, which type of funding: doctoral school, ANR submitted

Monte-Carlo simulations of alloying effects in the growth of 2D materials

The recent discovery of two-dimensional materials (2DMs) has revolutionized solid-state physics thanks to their ability to confine carriers. Since the discovery in 2004 of graphene, these materials have aroused an ever-growing interest since different materials form 2D layers: carbon, silicon, transition metal dichalcogenides... Graphene has shown remarkable properties, such as the Dirac-cone-shaped energy band and high carrier mobility. However, despite significant efforts, there has been no reproducible method to open up its bandgap while preserving high carrier mobility. 2DMs based on group IV elements such as Si (silicene) and Ge (germanene) are promising alternatives. Manufacturing good quality, quality-controlled such 2D crystals is thence of major importance from both fundamental and applied perspectives. Their growth by epitaxy that is both the fundamental cleanest way and a technological lock is thence the focus of different experimental studies. The growth on some metallic substrates revealed possible alloying effects that need to be understood and controlled. The goal of this internship is to advance in the theoretical understanding of these systems by using kinetic Monte-Carlo simulations that is the most suitable tool to describe these systems over the relevant space and time scales.

The numerical part will include the derivation of a rejection-free kinetic Monte-Carlo following the Bortz-Kalos-Lebowitz algorithm. The latter is suitable for simulations where transition rates are all known initially. We will study an on-lattice solid-on-solid (SOS) model that describes a crystal without voids and allows to simplify the description of atomistic vibrations. This model will include different atomic events starting with the fundamental deposition, diffusion and attachment/detachment processes. These processes will be made dependent on different configurations (local height, local configuration …) to account for different effects (segregation, alloying, wetting etc). Kinetic energy barriers are crucial parameters in kinetic Monte-Carlo simulations, and their absolute values may trigger different regimes (e.g. with fractals or compact growth shapes as a function of the nearest-neighbour interactions). Hence, we will consider first typical values for these barriers, already derived in some experimental studies (e.g. 2D flakes densities, shapes, amount of alloying etc) and first-principles calculations (e.g. considering energy barriers in energy landscapes). We will then systematically analyse the outcomes of the simulations depending on these barriers and will compare with experimental results in order to derive typical values and bounds. The aim of this coupling between theory and experiment is to gain control on the growth procedure in order to obtain two-dimensional epitaxial deposits of large size and good crystalline quality. The internship will be done in close collaboration with the experimental group at INSP that precisely performs epitaxial growth of silicene and germanene e.g. on Ag(111).



Condensed Matter Physics: YES	Soft Matter and Biological Physics: YES
Quantum Physics: NO	Theoretical Physics: YES