Doctoral positions
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Thesis topic Theoretical study of the growth of core-shell nanowires

Nanowires (NW) are under active scrutiny due to their importance for both fundamental science and technological applications. On one hand, they challenge the understanding of the basic mechanisms in crystal growth and of out-of-equilibrium statistical physics. On the other hand, they offer unique transport and optical properties resulting from the one-dimensional confinement [ZwanDzur13]. The dependence of their physical properties on their morphology, structure and composition is critical and requires a deep and precise investigation. If most studies dealt with single material NW, we aim at studying core-shell nanowires (see Fig. 1) that offer unique possibilities, such as a change from indirect to direct band-gap in Silicium-Germanium systems [ZhanDave11].

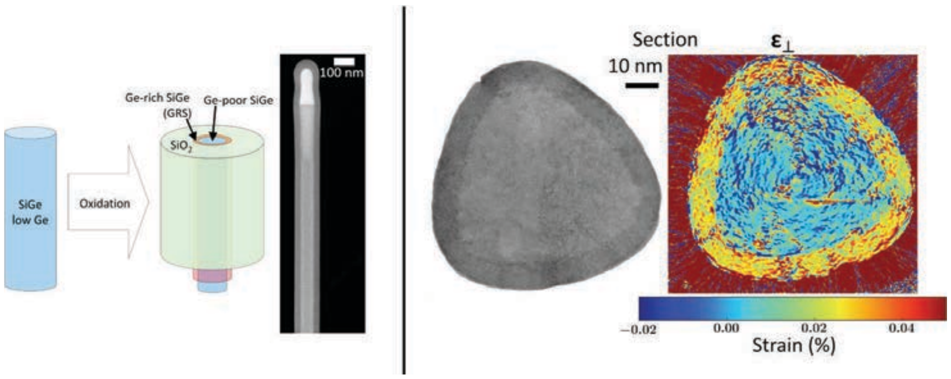

Fig. 1 : Core-shell nanowires made by molecular beam epitaxy [DaviLiu17]

The goal of this thesis is to study theoretically the growth of core-shell nanowires. The growth of these nano-objects now mainly proceeds via deposition in a vacuum environment in the so-called epitaxial mode. It is dictated by dynamical effects associated with atomistic processes such as deposition, diffusion, and nucleation, and, in nanowires, by geometry. First, the nanowire cylindrical geometry controls the surface diffusion process. Second, the core-shell structure with two different materials with different lattice parameters, generates elastic interactions that propagate throughout the system and build an explicit dependence on the geometry.

To understand the growth of these systems, one needs to describe the dynamical evolution dictated by surface diffusion. It can be done in a continuum framework that describes both capillarity and elasticity. In thin films on a flat substrate, it reveals the existence of an instability, which non-linear evolution eventually leads to the self-organization of quantum dots, in very good agreement with observations [AquaGouy13].

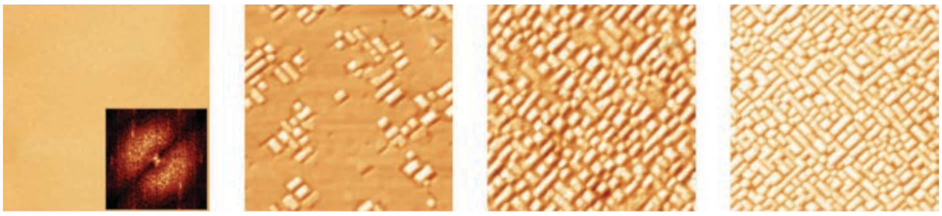

Fig. 2 : Comparison experiments / theory for the growth of strained quantum dots [AquaGouy13] on a flat substrate

To describe core-shell nanowires, one will first characterize the elastic interactions in the geometry under scrutiny. This may be done using a decomposition over the appropriate eigenfunctions of the equilibrium equations. The long range of elastic interactions leads to a subtle and rich interplay between geometry and dynamics [AquaXu14,ZhanAqua16]. The evolution of the surface at large time, where quantum dots arise on the shell, will then be investigated using possibly one or two frameworks. The first one corresponds to the non-linear description of the dynamical evolution. The second one corresponds to kinetic Monte-Carlo simulations that should describe a nucleation-driven evolution. Of special interest is the possible correlation between dots localization due to the long-range strain field that propagates through the wire. The growth of quantum dots on the nanowire shell will be compared with experiments using a novel growth technique dedicated to the investigation of core-shell nanowires in a collaborating experimental group [DaviLiu17].

References:

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