Internship proposal for a second-year master student

Electric-field-assisted growth of crystal-phase quantum dots: an *in situ* TEM study

Duration: 6 months starting from mid-March
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Context of the project: Growth of III-V semiconductor nanowires (NWs) using the vapour-liquid-solid (VLS) method can result in crystal structures different from their bulk phase [*1*]. In GaAs NWs, for example, stable zincblende (ZB) phase coexists with metastable wurtzite (WZ) structure resulting in NWs having a mixed-phase structure. Remarkably, the valence and conduction bands of the two phases are misaligned so that small sections of one phase within the other effectively confine charge carriers. Controlled switching between the two phases enables the synthesis of novel heterostructures, crystal-phase quantum dots (CPQD), with exceptional properties and potential applications in photonics [*2,3*] and quantum computing [*4*]. In contrast to compositional heterojunctions, **CPQDs have intrinsically abrupt interfaces and hence do not suffer from the alloy intermixing at the interface**, which hampers precise control of the electronic properties in compositional heterostructures.

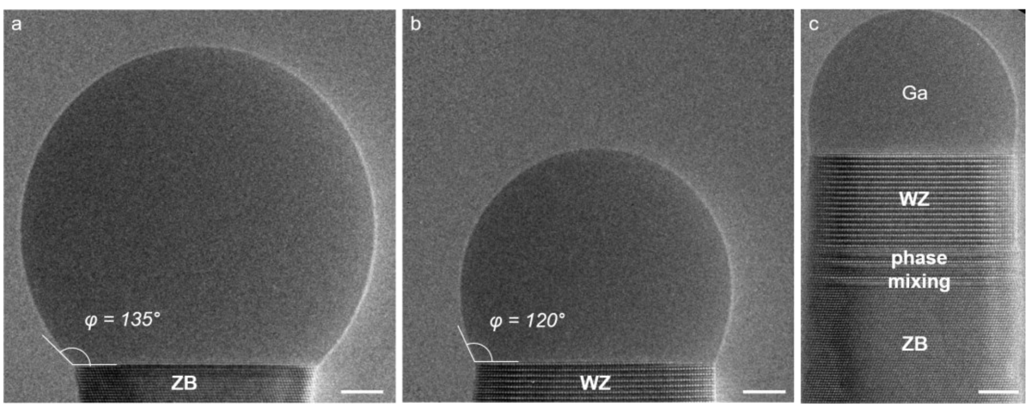

Figure 1. Impact of contact angle on the phase selection [*9*]. Images of a self-catalyzed GaAs NW recorded using the NanoMAX *in situ* TEM. The NW was grown by molecular beam epitaxy using the vapor-liquid-solid (VLS) method, where a liquid metal droplet (Ga in this case) catalyzes the growth of a solid NW from material provided from a gas phase. The As/Ga flux ratio was changed during growth to tune the volume of the catalyst droplet and, consequently, the contact angle, φ. A large contact angle ($\varphi > 125°$) results in the growth of ZB (**a**), while a small one corresponds to WZ (**b**). **c** shows the phase mixing at the interface between the two phases. Scale bars are 5 nm.

Even though CPQDs were first discovered more than ten years ago, their technological application has been severely limited by the difficulty of needing precise control over their growth. In particular, the physics underlying the phase selection mechanism was poorly understood, and so the studies investigating the optical properties of CPQDs were mainly relying on accidentally formed CPQDs [*2*]. Only recently, thanks to *in situ* transmission electron microscopy (TEM), we started to shed light on this mechanism. *In situ* TEM provides unparalleled imaging resolution and allows the capturing of the growth dynamics [*5*,*6*,*7*] and the effect of growth parameters in real-time. Using this technique, we demonstrated that **the sole parameter determining the phase selection is the contact angle** between the droplet and the NW interface (Figures 1a and 1b) [*8,9*]. Up to now, the only way to change the contact angle was by modifying the droplet volume by changing the growth conditions. This process is extremely difficult to control, and in most cases, it generates a segment of mixed phases at the interface between WZ and ZB (Figure 1c). Ideally, we would need a method to change the contact angle instantaneously, without modifying the growth conditions. Luckily, such a method exists and consists of applying an electric field parallel to the growth direction. **The electric field deforms the droplet, directly altering its shape and contact angle without affecting other aspects of growth**. We explored this concept using Au-catalyzed Si NWs, and demonstrated that it is a viable method to precisely control the droplet contact angle [*10*] (Figure 2).

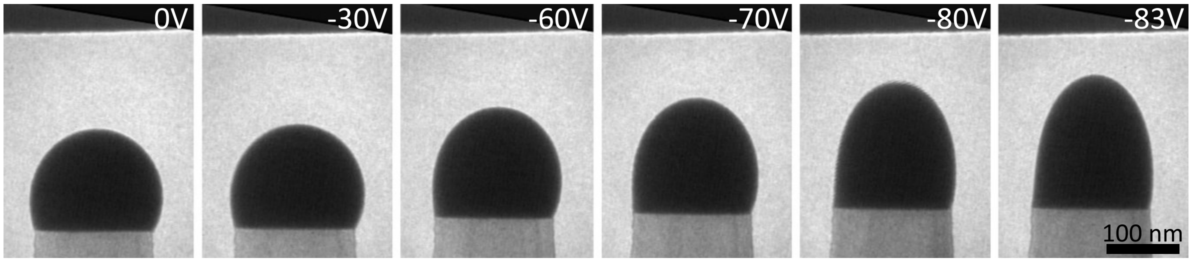

Figure 2. Droplet deformation using an electric field [*10*]. Image sequence showing the electric-field- induced deformation of the catalyst droplet on a Si NW.

The aim of this project is to use an electric field to modify the contact angle of GaAs NWs to achieve unprecedented control over the crystal phase. This method will be used to create multiple CPQDs of controlled dimensions and spacing. This result will be achieved in several steps: (1) micro-fabrication and characterization of microelectromechanical systems (MEMS) samples. (2) Study of the electric-field-induced phase switching using *in situ* TEM. (3) Modeling of the growth mechanism. (4) Transfer of the method developed *in situ* to a metal-organic chemical vapor deposition (MOCVD) reactor. (5) Study of the physical properties of the fabricated CPQDs. The *in situ* experiments will be conducted using the MOCVD growth method in the NanoMAX TEM [9]. The physical properties of the obtained heterostructures will be investigated by photoluminescence (PL) and cathodoluminescence (CL).

Master 2 internship: The goal of this internship is to develop the data analysis tools for the *in situ* electric-field experiments. The student will participate in the experiments, and he/she will be in charge of data analysis and basic modeling. The analysis will be carried out by developing an automated image-processing algorithm able to extract relevant geometric parameters (i.e. droplet size, contact angle, crystal phase) from each image. The resulting data will be used to correlate the changes of contact angle to phase switching and develop a model to determine E-field's effect on the growth of GaAs nanowires.

Continuation to Ph.D.: This work could be extended to a Ph.D. thesis. The applicant will design, fabricate and characterize a new generation of MEMS-based samples to improve the control of electric field and temperature during the growth of nanowires. He/she will then actively participate in the *in situ* experiments aimed at understanding the electric-field-induced phase switching mechanism and determine the ideal conditions (i.e. pressure, temperature, E-field) to apply this method on a full-wafer scale in a standard MOCVD reactor.

Candidate profile: Highly motivated candidates enrolled in a master's degree or equivalent, with a background in materials science and/or physics. Prior knowledge in crystal growth, programming or other fields that are relevant to the project would be appreciated.

Application procedure: For additional information about the project and/or the recruitment process, please contact Federico PANCIERA (federico.panciera@c2n.upsaclay.fr). The candidate should include a CV and at least one recommendation letter.

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