Internship proposal for a second-year master student

In situ TEM study of crystal-phase heterostructures in III-V nanowires

Duration: 6 months starting from March
Salary 600 EUR/month
Supervisor: Federico PANCIERA
Laboratory: Centre for Nanoscience and Nanotechnology (C2N), U. Paris-Saclay/CNRS
Web: https://panciera.netlify.com, https://elphyse.c2n.universite-paris-saclay.fr/en/
Contacts: federico.panciera@c2n.upsaclay.fr

Context of the project: Semiconductor nanowires (NWs) exhibit unique properties that make them potential building blocks for a variety of next generation devices such as biosensors, solar cells, transistors, quantum light sources and lasers. In order to take advantage of the physical properties of NWs, it is crucial to control their geometry, crystal structure and doping. This goal will ultimately be achieved by a deep understanding of the growth mechanisms. The most common growth technique is the vapor-liquid-solid (VLS) method, where a liquid metal droplet catalyzes the growth of a solid NW from gas phase precursors. In this growth mode, the droplet plays a fundamental role in determining the structure of the nanowire, and the remarkable range of structures enabled by VLS can be thought of as the result of engineered changes to the droplet.

For example, growth of III-V semiconductor NWs using the VLS method can result in crystal structures different from their bulk phase [*1*]. In GaAs NWs 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 alloy intermixing at the interface**, which hampers precise control of the electronic properties in compositional heterostructures.

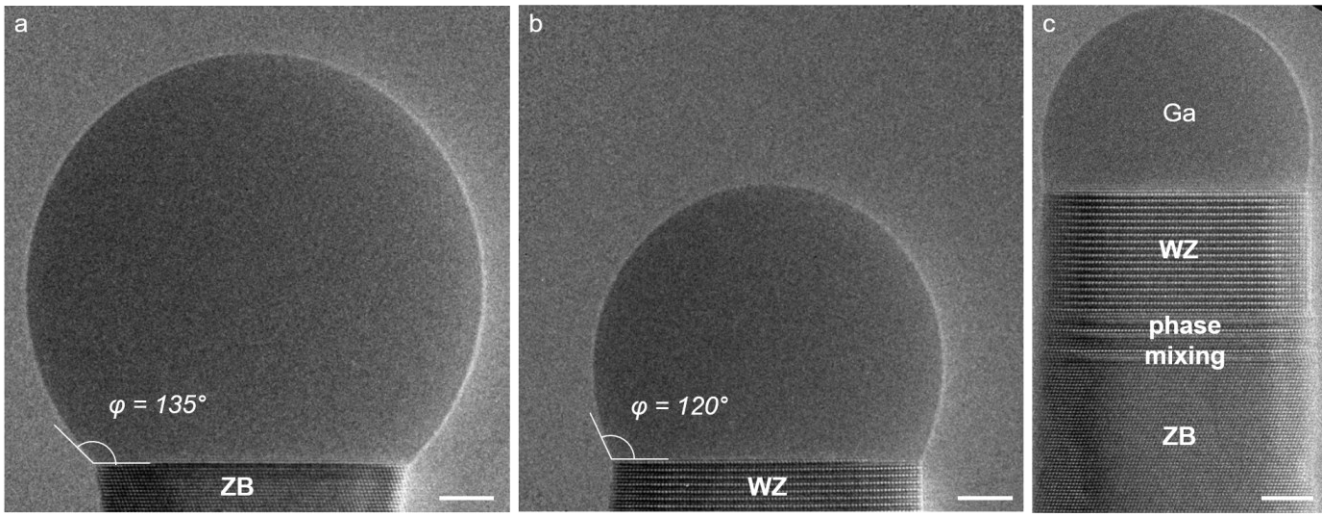

Figure 1. Impact of contact angle on the phase selection [*9*]. Images of a self-catalyzed GaAs NW recorded using the NanoMAX *in situ* TEM. The NW was grown by molecular beam epitaxy using the vapor-liquid-solid (VLS) method, where a liquid metal droplet (Ga in this case) catalyzes the growth of a solid NW from material provided from a gas phase. A large contact angle (φ > 125°) results in the growth of ZB (**a**), while a small one corresponds to WZ (**b**). **c** Shows a NW having segments of the phases. Scale bars are 5 nm.

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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. 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) [*8,9,10*].

The aim of this project is to develop strategies for the control of the contact angle of GaAs NWs to achieve unprecedented control over the crystal phase.

Master 2 internship: The successful applicant will actively participate in the *in-situ* experiments and will be in charge of the data analysis. The *in situ* experiments will be conducted using the MOCVD growth method in the NanoMAX TEM [9]. The analysis will be carried out by developing dedicated image-processing algorithms 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 predict the crystal phase for different growth conditions.

This work could be **extended to a Ph.D**. funded by the ANR project ELEPHANT.

Candidate profile: Highly motivated candidates enrolled in a master's degree or equivalent, with a background in physics, materials science or engineering. Prior knowledge in programming (possibly Python) would be highly 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.

References

[1] Algra et al. Twinning superlattices in indium phosphide nanowires. *Nature* **2008,** *456* (7220), 369-372.

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[4] Hastrup et al. All-optical charging and charge transport in quantum dots. *Scientific Reports* **2020,** *10*(1), 1-6.

[5] Ross, F.M. Controlling Nanowire Structures through Real Time Growth Studies. *Reports Prog. Phys.* **2010**, *73*(11), 114501.

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[9] Panciera et al. Phase selection in self-chatalyzed GaAs nanowires. *Nano Lett.* **2020**, *20*(3), 1669-1675.

[10] Panciera et al. Controlling nanowire growth through electric field-induced deformation of the catalyst droplet. *Nature communications*, **2016**, *7*(1), 1-8.