

Wurtzite phase control of self-assisted GaAs nanowires grown by molecular beam epitaxy

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III-V semiconductor nanowires (NWs) obtained by the vapor-liquid-solid mechanism exhibit a zinc-blende (ZB) or a wurtzite (WZ) structure depending on the growth conditions, and more particularly on the amount of III and V element fluxes. Nevertheless, the optimized molecular beam epitaxy (MBE) growth of WZ segments in NW geometry is still in its infancy, and major achievements have been reported only very recently. In this work, we used an analytical growth model to show the existence of a stationary regime allowing the formation of pure WZ phase, by precisely tuning the V/III flux ratio. The combination of RHEED evolution with high-resolution STEM and dark field TEM confirmed the MBE growth of a micron-long pure WZ segment, in self-assisted GaAs NWs.

Keywords: self-assisted nanowires, molecular beam epitaxy, wurtzite, VLS, GaAs, wetting angle

III-V semiconductor nanowires (NWs) obtained by the vapor-liquid-solid (VLS) mechanism exhibit a zinc-blende (ZB) or a wurtzite (WZ) structure¹ depending on the growth conditions, and more particularly on the amount of III and V element fluxes². While it has been reported that self-assisted GaAs NWs crystallize mostly in the ZB phase, their gold-catalyzed counterparts essentially lead to the WZ structure. Given the advantages of molecular beam epitaxy (MBE) for the synthesis of high purity crystals and control of deposited thickness down to the atomic monolayer level, controlling precisely the growth of the WZ crystal phases in self-assisted GaAs NWs by molecular beam epitaxy (MBE) thus appears to be a relevant challenge to address for device applications³. Nevertheless, the optimized growth of WZ segments in NW geometry is still in its infancy, and major achievements have been reported only very recently⁴⁻⁷.

Here, we used an analytical growth model to demonstrate the existence of a stationary regime allowing the formation of a pure WZ phase, by a precise tuning of the V/III flux ratio. A slight change in the As flux indeed induces a modification of the catalyst droplet wetting angle in a desired range of values, which can be maintained to form extended pure WZ segments. The combination of *in situ* reflection high energy electron diffraction (RHEED) evolution with high-resolution scanning transmission electron microscopy (STEM) and dark field TEM, as well as photoluminescence, confirmed the successful control of a pure WZ segment, more than a micrometer long, obtained by MBE growth of self-assisted GaAs NWs with a V/III flux ratio of 4.0⁸.

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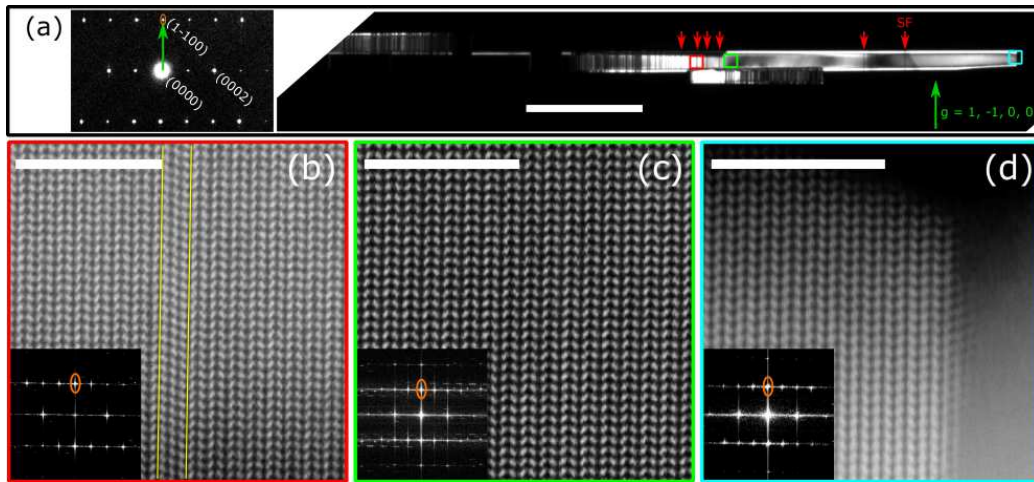


Figure 1: (a) DF-TEM image of the extended WZ segment. The red arrows indicate the stacking faults visible in the WZ segment. Scale bar: 500 nm. High-resolution STEM-HAADF images showing (b) the beginning of the extended WZ segment with a 3 monolayers long ZB segment, (c) a portion of the extended WZ segment and (d) the end of the extended WZ segment with the Ga droplet/NW interface. (b) - (d) Correspond to the regions highlighted with colored squares, red, green and cyan, respectively, in (a). The WZ spots of the FFT are highlighted with the orange circles, respectively. Scale bars on (b) - (d) are 5 nm.