The Zincblende/Wurtzite Interface in III-V Nanowires: Heterostructures with Atomically-abrupt Electronic Transition

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III-V semiconductor nanowires (NWs) have a large technological potential within energy harvesting and (opto)electronics [1]. In addition, they provide a unique playground in materials science, since their small footprint allows the formation of a wide range of radial and axial heterostructures with changes in material composition, doping, or crystal phase. Recently, it became possible to purposely tune the crystal structure between Zincblende (Zb) and Wurtzite (Wz) phase over InAs or GaAs NW segments of varying length [2].

Here, we use low-temperature scanning tunneling microscopy and spectroscopy (STM/S) to monitor both the atomic surface structure and the surface local density of states (LDOS) across Zb/Wz interfaces in InAs NWs. The NWs include Zb and Wz segments of varying length, down to the shortest possible insertion of Zb phase in a Wz matrix, i.e. a Zb single bilayer stacking fault. We compare STS spectra obtained at As atoms in the stacking fault with spectra from As atoms located 1 nm, 3 nm, and 5 nm away from it. Thereby we find similar Wz LDOS signal further away and in close proximity to the stacking fault, while the stacking fault itself shows a clear Zb signature. These results demonstrate that the atomically sharp structural transition between Zb and Wz phase is accompanied by an equally abrupt electronic transition. In addition, we analyze conduction band and valence band onsets from STS results obtained at Wz segments with Zb inclusions of varying length. We obtain strong valence band offsets and a nearly flat conduction band, in agreement with previous results on extended Wz and Zb segments [3], and we observe confinement energies of up to 30 meV with decreasing length of the Zb segment.

Furthermore, we present initial tests on utilizing NWs with Wz and Zb segments for the creation of advanced 3D heterostructures with atomic precision: We expose GaAs NWs with both Wz and Zb segments to Sb and monitor the incorporation of individual Sb atoms in the surface due to Sb-for-As exchange reactions. Thereby we find a preferential incorporation of Sb in the Zb {110} surface facets, as compared to Wz {11-20} surface segments (see Fig. 1), which is also verified by density functional theory calculations [4]. Such preferential incorporation, prior to subsequent radial overgrowth, opens up a path towards atomically thin quantum rings of tunable diameter and height.

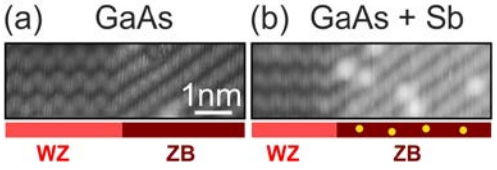

Figure 1: *STM images of a GaAs Wz/Zb surface (a) before and (b) after Sb exposure. Bright spots in (b) are individual Sb atoms.*

[1] J. Wallentin et al., Science 339, 1057 (2013); E. Lind et al., IEEE J. El. Dev. Soc. **3**, 96 (2015).
[2] S. Lehmann et al., Nano Lett. **13**, 4099 (2013). [3] M. Hjort et al., ACS Nano **8**, 12346 (2014).
[4] M. Hjort et al., Nano Lett. **17**, 3634 (2017).

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Supplementary Page (Optional)

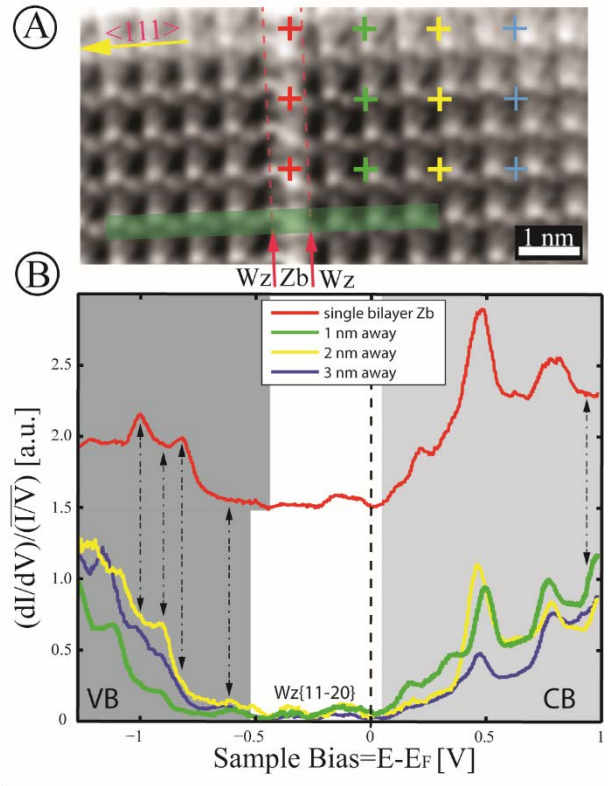

Figure 2:
(A) STM image of a Wz {11-20} surface segment of an InAs NW with a Zb single bilayer stacking fault. (B) STS spectra, averaged over positions of the same color indicated in (A), showing the normalized differential conductance. Energies where the spectra acquired at the Zb stacking fault (red curve) show significantly different behavior than those acquired at the Wz surface (green, red, and blue curves) are indicated by black arrows. The position of the valence band (VB) and conduction band (CB) is overlaid in dark and light grey.

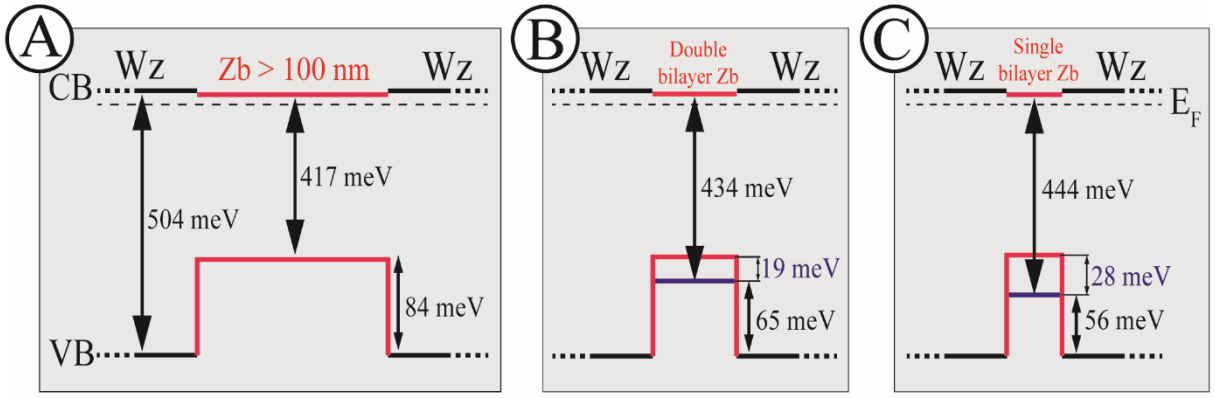

Figure 3: Energy diagram showing the conduction band (CB) and valence band (VB) onset of Wz and Zb segments in InAs NWs, as obtained from STS spectra acquired at 5K. For double and single bilayer Zb stacking faults, confined states with a confinement energy of 19 meV and 28 meV are observed.