

## Investigation of GaAs-based nanowire heterostructures using tomography based on STEM-HAADF tilt-series[1]

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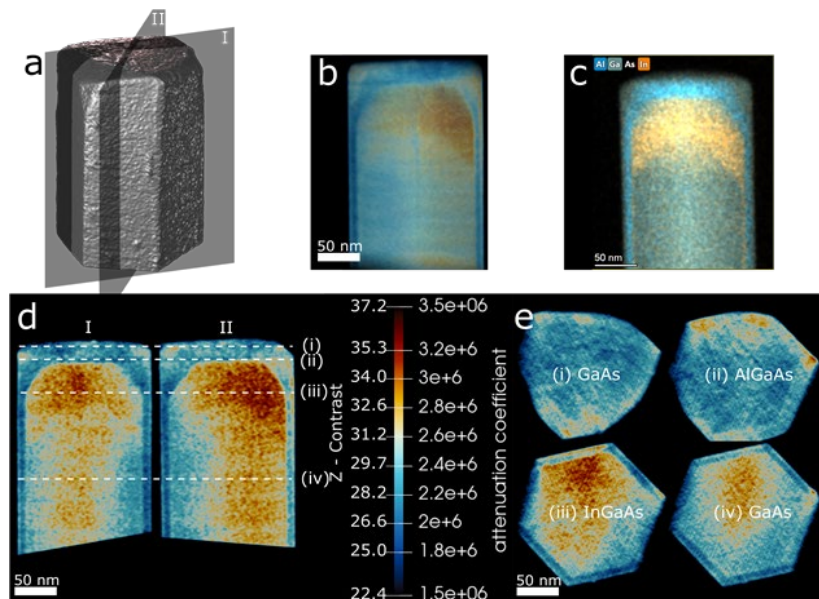
In the development of on-chip electronics, group III/V semiconductor nanowires (NWs) hold great interest, due to their small footprint allowing compatibility with lattice mismatched substrates like silicon while greatly increasing the chemical flexibility.[2] Within this work GaAs-NWs with optically active axial InGaAs heterostructures and an AlGaAs capping layer are investigated. These spatially confined optical cavity structures facilitate low loss propagation of optical modes and show a high refractive index contrast.[3] We aim to create a better understanding of the exact structure and the resulting structure property relationship of the InGaAs heterostructure based on previously measured low-temperature photoluminescence spectra.[1]. As the functionality of these heterostructures, like efficient carrier confinement, is closely linked to their 3D structure and chemical composition, tomographic reconstructions employing STEM HAADF tilt-series were carried out. To this end a tilt series with a tilt range from  $-75^\circ$  to  $75^\circ$  was measured on a probe corrected FEI Titan Themis electron microscope and reconstructed using a weighted SIRT algorithm as well as finite support correction after preprocessing and alignment. The resulting tomogram is shown as an isosurface in Figure 1a. It consists of six sidewall facets perpendicular to the main [111] growth direction terminating in a flat capping layer. Assuming Lambert-Beer's law, the obtained attenuation coefficients can be qualitatively correlated to atomic numbers by using two reference areas of the tomogram, here AlGaAs (Al and Ga assumed to be 1:1) and GaAs neglecting the very low Sb concentration. As the Z-contrast shows the average atomic number of the elements present, AlGaAs was set to  $Z = 27.5$  and GaAs set to  $Z = 32$  respectively.

This assumes the small differences in crystal parameters between AlGaAs and GaAs are neglectable. The resulting element mapping corresponds well with the elemental compositions obtained from EDX, as can be seen by comparing Figure 1b and the corresponding EDX data acquired in the same projection direction in Figure 1c. While the facets are well measured some missing wedge artifacts and a slight density gradient based on the unaccounted carbon support are still present as seen in the slices along the growth direction shown in Figure 1e. The threefold faceted capping layers as seen in Figure 1e(i) show a truncated tetrahedral growth governed by the threefold

symmetry of the ZnS type crystal structure of GaAs in combination with twinning defects. In order to validate the use of the Lambert-Beer-Law for STEM HAADF measurements, pytorch multi-slice simulations were conducted for GaAs at different tilt angles using the frozen phonon approximation to account for thermal diffuse scattering, and compared to the experimental results. Furthermore, the possibility to reducing the artifacts resulting from the missing wedge focus series are investigated by multi-slice simulations and experiments.

Figure 1: STEM tomographic analysis of the GaAsSb/InGaAs/AlGaAs NW heterostructure; (a) 3D isosurface rendering of the NW tip, illustrating the facet structure consisting of six sidewall facets perpendicular to the [111] growth direction. (b) Z-contrast volume rendering of the NW, (c) corresponding EDXS map of the same NW with comparable color code, (d) two central cuts parallel to {1-10} sidewall facets (as indicated in (a)), exposing the Z-contrast through the core. (e) Cross-sections at different positions along the NW (as indicated in (d) by labels (i)-(iv)), revealing the Z-contrast in radial direction from top (GaAs) to bottom (GaAsSb) of the NW heterostructure.

**Graphic:**



**Keywords:**

Nanowires, Tomography, STEM, Simulations, GaAs

**Reference:**

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