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The Outward Diffusion of Sb during Nanowire Growth Studied by Quantitative High-Angle Annular Dark Field Scanning Transmission Electron Microscopy.

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Planar antimony (Sb) containing compound semiconductors are used in a broad range of optoelectronic devices. The optical properties of these devices can be tailored by the Sb concentration. In the case of Sb containing nanowires (NWs) the high surface-to-volume ratio can affect the Sb composition control during the NW growth. In previous studies on both Au- and Ga-assisted molecular beam epitaxy (MBE) grown $GaAs_{1-y}Sb_y$ inserts in GaAs NWs, a reduction in the Sb concentration towards the outer surface was found [1, 2]. The radial composition variations could be caused by i) As-Sb exchange at the surface and/or ii) radial GaAs overgrowth during NW growth.

In order to understand the origin for the observed radial compositional variations, we have systematically studied the radial Sb distribution in MBE grown Ga-assisted $GaAs_{1-y}Sb_y$ NWs as well as in axial $GaAs_{1-y}Sb_y$ inserts (50-150 nm long) in both Ga- and Au-assisted GaAs NWs (Fig. 1). The Sb distribution was studied by quantitative high-angle annular dark field scanning transmission electron microscopy (HAADF STEM) on as-received NWs, i.e., no additional specimen preparation was applied. All experiments were performed on a non-corrected TEM/STEM at medium magnifications.

The experimental HAADF STEM intensities were normalized to the incident beam intensity to allow for direct comparison with simulated intensities from frozen-lattice multislice simulations [1,3]. The simulations included static atomic displacements, as well as the increase in the unit cell size and the Debye-Waller factor of Ga due to alloying with Sb. For pure zinc blende (ZB) and wurtzite (WZ) GaAs segments and GaAsSb segments near the catalytic droplet experiments and simulations displayed a nearly perfect fit indicating a radially homogeneous composition (Fig. 2(a)).

In the case of GaAsSb NWs, an increased reduction of Sb at the surface with increasing growth time was observed. In the HAADF STEM intensity profiles across the NWs this was observed as an increasing deviation from the simulated intensity profiles assuming a homogeneous radial Sb distribution when moving from the tip towards the bottom of the NW. The experimental HAADF STEM profiles could be explained using a diffusion model with endless Sb sink at the outer surface due to As-Sb exchange during growth (Fig. 2(b)).

In the case of the GaAsSb inserts an even more pronounced deviation from the simulated intensity profile assuming a homogeneous Sb distribution was observed. This could be explained by a combined effect of radial GaAs overgrowth and diffusion of Sb into the overgrown GaAs layer (Fig. 2(c,d)). The radial distribution profiles are different for the Ga- and Au-assisted growth as the growth temperatures are different.

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As the initial HAADF simulations assumed a homogeneous Sb distribution in the direction of the electron beam, the presence of a reduced Sb content towards the outer surface might have led to an underestimation of the Sb content based on quantitative STEM. Using different diffusion models developed for these hexagonal-shaped nanowires for the different growth scenarios applied, the maximum Sb concentration (C_0) in the core of the NW could be estimated (Fig. 2). These deducted maximum Sb concentrations were compared to the initial quantitative STEM results and energy dispersive spectroscopy measurements on the same NWs. Tentative intensity simulations based on inhomogeneous Sb profiles were performed to estimate the inaccuracy. The effect of the inhomogeneous radial Sb distributions on the optoelectronic properties is discussed.

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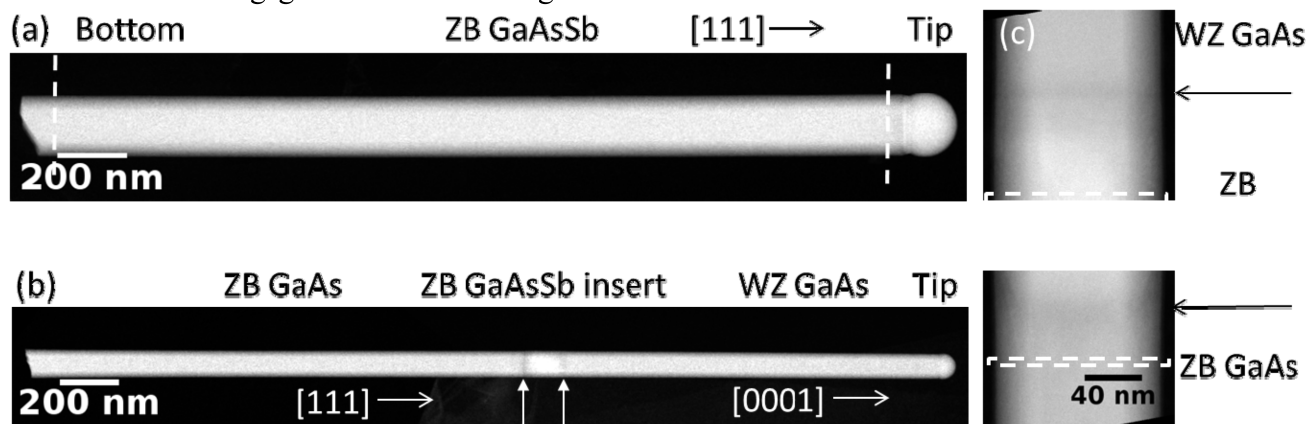

Figure 1. HAADF STEM images of (a) a Ga-assisted GaAsSb NW, (b) a Ga-assisted NW with GaAsSb insert, indicated by arrows, and (c) the insert in (b) at a higher magnification. Profiles across ZB GaAs and GaAsSb are marked by dashed lines and boxes.

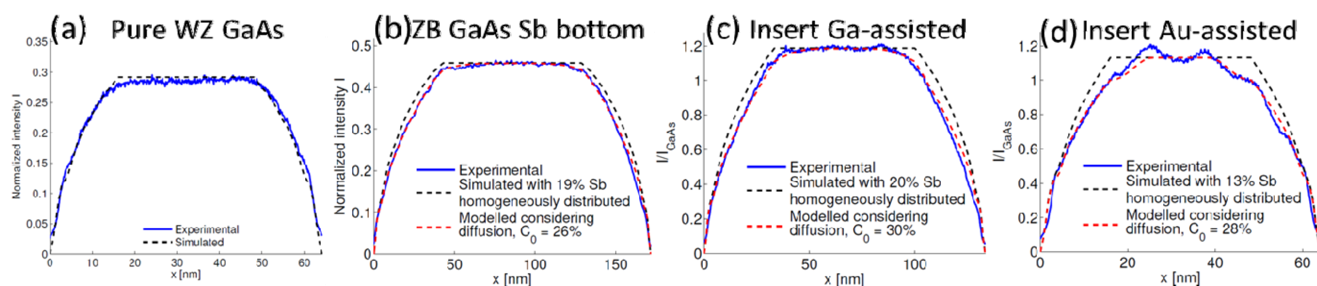

Figure 2. Example intensity profiles of (a) pure WZ GaAs reference region, (b) at the bottom of a GaAsSb NW, (c) at the center of a GaAsSb insert in Ga-assisted NW and (d) at center of a GaAsSb insert in Au-assisted NW. Blue is the experimental intensity profile, black dashed line is the simulated profile (assuming homogeneous Sb distribution) and red dashed line is the modelled profile, taking diffusion (b-d) and GaAs overgrowth (c,d) into account. The profiles are normalized to the electron beam (a,b) or GaAs reference area (c,d).

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