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# InAs nanowires with $Al_xGa_{1-x}Sb$ shells for band alignment engineering

ABSTRACT



CRYSTAL GROWTH

Torsten Rieger\*, Detlev Grützmacher, Mihail Ion Lepsa

Peter Grünberg Institute and JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

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InAs nanowires surrounded by  $Al_xGa_{1-x}Sb$  shells exhibit a change in the band alignment from a broken gap for pure GaSb shells to a staggered type II alignment for AlSb. These different band alignments make  $InAs/Al_xGa_{1-x}Sb$  core-shell nanowires ideal candidates for several applications such as TFETs and passivated InAs nanowires. With increasing the Al content in the shell, the axial growth is simultaneously enhanced changing the morphological characteristics of the top region. Nonetheless, for Al contents ranging from 0 to 100 % conformal overgrowth of the InAs nanowires was observed. AlGaSb shells were found to have a uniform composition along the nanowire axis. High Al content shells require an additional passivation with GaSb to prevent complete oxidation of the AlSb. Irrespective of the lattice mismatch being 1.2% between InAs and AlSb, the shell growth was found to be coherent.

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## 1. Introduction

The combination of different semiconductor materials into lowdimensional heterostructures offers new possibilities ranging from fundamental physics [1] to devices being suitable for "More than Moore". For the latter, especially tunnel field effect transistors (TFETs) are considered as ideal candidates since they allow a subthreshold slope of less than 60 mV/dec with a high on and low off current [2]. Here, TFETs make use of either a staggered or even a broken band alignment. III-V semiconductors belonging to the 6.1 Å family (InAs, GaSb and AlSb) cover the different types of band alignment [3] and are therefore suitable materials for TFETs. Additionally, the low lattice mismatch ( $\leq$  1.2%) results in low dislocation density or even coherent growth. Taking such devices into the nanowire (NW) geometry should even enhance the region of coherent growth due to improved strain accommodation [4]. Applying classical Matthews–Blakeslee theory [5] to InAs/GaSb and InAs/AlSb results in critical thicknesses of 20 nm and 10 nm, respectively.

While several NW-TFET devices based on the broken gap InAs/ GaSb system have been demonstrated [6,7], staggered InAs/AlGaSb TFETs have been limited to planar structures [8,9]. However, Knoch and Appenzeller [10] showed that the staggered band alignment with an Al content of about 60% should result in the best performance. Considering InAs NWs embedded in high Al content shells, the large electron barrier of up to 1.35 eV can significantly enhance the electron mobility due to reduced surface scattering [3,11,12]. Therefore, this insitu passivation of InAs NWs with an almost lattice matched shell is of particular interest for high-mobility devices. In this context, we present the growth, morphological and structural analyses of  $InAs/Al_xGa_{1-x}Sb$  core-shell NWs with Al contents varying from 0 to 100% using molecular beam epitaxy.

### 2. Experimental details

Si (111) substrates were cleaned in hydrofluoric acid to remove the native oxide and absorbents. A thin silicon oxide was subsequently prepared wet chemically by placing the samples for 60 s in hydrogen peroxide. Hereafter, they were loaded into the molecular beam epitaxy (MBE) system and degased at 200 °C and 400 °C in the load lock and buffer chamber, respectively. After introduction in the MBE chamber, additional outgasing at 600 °C takes place and subsequently, the temperature was lowered to the growth temperature of the InAs NWs being 490 °C. Vapor solid InAs NWs were grown with an In rate of  $0.035 \,\mu\text{m/h}$  and an As<sub>4</sub> beam equivalent pressure of  $10^{-5}$  mbar for 1 h [13]. Hereafter, the substrate temperature was decreased to 360 °C keeping the As shutter open. After reaching this temperature, the As shutter was closed and the Sb shutter was opened 2 min prior to the Ga and Al shutters. The Sb flux was set to  $7\times 10^{-7}$  mbar and the total flux of the group III elements was kept constant at a planer growth rate of 0.1  $\mu$ m/h. If not mentioned differently, the growth duration of the shell was 60 min resulting in shell thicknesses of  $\sim$  20–25 nm. These growth conditions have been previously determined to be optimal for GaSb shells covering InAs NWs [14]. Considering planar growth, the critical thickness according to Matthews-Blakeslee is 20 nm for GaSb and decreases to 10 nm for AlSb.

The grown samples have been analyzed by scanning and transmission electron microscopy (SEM and TEM). In the latter

<sup>\*</sup> Corresponding author. Tel.: +49 2461 61 2732; fax: +49 2461 61 2333. *E-mail address:* t.rieger@fz-juelich.de (T. Rieger).

one, also energy dispersive x-ray spectroscopy (EDX), selective area electron diffraction (SAED) and high angle annular dark field (HAADF) have been used. High resolution TEM (HRTEM) images were filtered by applying a mask to the fast Fourier transform (FFT) maintaining solely the {111} lattice planes.

#### 3. Results and discussion

Fig. 1 shows overview SEM micrographs of InAs/Al<sub>x</sub>Ga<sub>1-x</sub>Sb core-shell NWs with x ranging from 0 to 1 in steps of 0.2. For all Al contents, the NWs have uniform dimensions, no clustering is observed. The only remarkable difference is found at the top of the NWs. For pure GaSb shells, a platform develops at the top, having a flat facet as well as a diameter expansion compared to the rest of the NW. The InAs NW itself does not have this flat facet but a rounded or tapered shape [14,15]. By increasing the Al content in the shell, the platform slowly vanishes and the flat top facet transforms into a rounded and faceted top similar to the pure InAs NW. The transition from a flat to a tapered shell occurs roughly in the region of 40-60% Al, however, it might also depend on the growth time of the shell. The flat top facet for GaSb shells can be attributed to a low growth rate of the {111}B facet compared to the {110} and {211} facets, the diameter expansion to radial growth occurring on zinc blende (ZB) GaSb inducing additional twins [14]. Contrary, when pure AlSb shells are grown, the growth rate of the {111}B facet is higher than that of the {110} and {211} facets. In this sense, using TEM micrographs the length of the axially grown GaSb was measured to be  $\sim$  0 nm while it increased to  $\sim$  50 nm,  $\sim$  80 nm and  $\sim$  95 nm for x=0.2, 0.6 and 1, respectively. Considering axial growth solely be caused by direct impingement, an axially AlGaSb segment of 100 nm would be expected. Thus, the presence of Al reduces the adatom mobility and therefore favors the axial growth of  $Al_xGa_{1-x}Sb$ .

The successful and homogenous incorporation of Al into the shells was confirmed by EDX line scans, two exemplary scans are shown in Fig. 2 together with bright field TEM images. Fig. 2a and b is taken from a core–shell NW with a nominal content of 20% Al. As can be seen, the Al signal in the EDX line scan is very weak, but

could be clearly identified in the spectra. The TEM image being acquired from the < 211 > zone axis shows very smooth surfaces and interfaces. No evidence of phase separation or an inhomogeneous alloy is found. The thickness of the native oxide of the Al<sub>0.2</sub>Ga<sub>0.8</sub>Sb shell is in the same range as that of pure GaSb shells, i.e., 3-4 nm. However, an increase of the Al content in the shell to 60% significantly increases the thickness of the native oxide being in the range of 8-10 nm (not shown). This is in fact a direct evidence for the incorporation of a higher amount of Al which has a stronger tendency for the formation of a native oxide laver. Consequently, an additional thin GaSb cap layer was grown around InAs/Al<sub>x</sub>Ga<sub>1-x</sub>Sb core-shell nanowires with Al contents above 20%. Fig. 2c and d depicts the TEM micrograph and corresponding EDX profile for an InAs/Al<sub>0.6</sub>Ga<sub>0.4</sub>Sb core-shell nanowire. As seen in the TEM image, the native oxide thickness is again in the order of  $\sim$ 4 nm and a corresponding delayed onset of the Al signal in the EDX profile is found. The Al/Ga is significantly higher than in Fig. 2b, thus the amount of incorporated Al in the shell increased. This not only proves that the thin GaSb shell prevents oxidation of the underlying AlGaSb, it is also a first demonstration of a multiple core-shell system based on arsenides and antimonides.

However, although the incorporation of Al into the shell is proven, the actual composition of the AlGaSb shell might vary along the growth axis. This can be caused by a temperature gradient along the nanowire axis [16,17] or different adatom diffusion lengths for Ga and Al. Consequently, EDX spectra were acquired at different positions along the nanowire axis of a coreshell nanowire with an Al<sub>0.6</sub>Ga<sub>0.4</sub>Sb shell. In order to compensate for thickness variations and sample drift, the intensities of Ga and Al were normalized to that one of Sb. The TEM micrograph, HAADF image as well as the corresponding EDX profile displayed in Fig. 3 show a uniform shell thickness along the NW axis as well as a relatively uniform composition. Slight variations should rather be caused by the limited time used to acquire the spectra than by a temperature gradient or differences in the adatom mobilities.

When pure AlSb shells are grown, the necessity of a GaSb cap preventing oxidation becomes even more evident. A pure, nominally 20 nm thick AlSb shell oxidizes completely if not protected by a GaSb cap. This can be clearly seen in the HAADF image in Fig. 4a with its



Fig. 1. SEM micrographs of InAs/Al<sub>x</sub>Ga<sub>1-x</sub>Sb core-shell NWs with Al contents of 0, 0.2, 0.4, 0.6, 0.8 and 1 in (a), (b), (c), (d), (e) and (f), respectively. All scale bars are 500 nm.

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