

Electronic supporting information

## Misfit dislocation free InAs/GaSb core-shell nanowires grown by molecular beam epitaxy

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### 1. Cross-sectional shape along the nanowire axis

The three dimensional morphology of the nanowires changes after covering the InAs core with the GaSb shell. As it is described in the main part of the manuscript, this morphological change can be investigated by means of SEM or HAADF profiles. Fig. S1a and b show SEM micrographs from the top and the bottom of an InAs/GaSb core-shell nanowire (shell growth at 360°C). Similar as discussed in the main part of the manuscript, multiple facets can be identified. However, the limited resolution of the SEM prohibits are more detailed investigation, especially at the very bottom and top of the nanowire. Thus, Fig. S1d depicts HAADF line profiles acquired at four different positions along the nanowire axis. The zone axis of the nanowire is  $\langle 110 \rangle$ . Following these profiles, the cross-sectional shape at the very bottom of the nanowire can be identified as hexagonal with  $\{211\}$  side facets. It is similar just below the GaSb platform at the top. However, taking a profile just slightly above the bottom/below the top modifies the cross-sectional shape strongly. It changes from a hexagonal shape to a dodecagonal shape with a combination of  $\{110\}$  and  $\{211\}$  side facets. This dodecagonal shape is maintained along the major part of the nanowire.

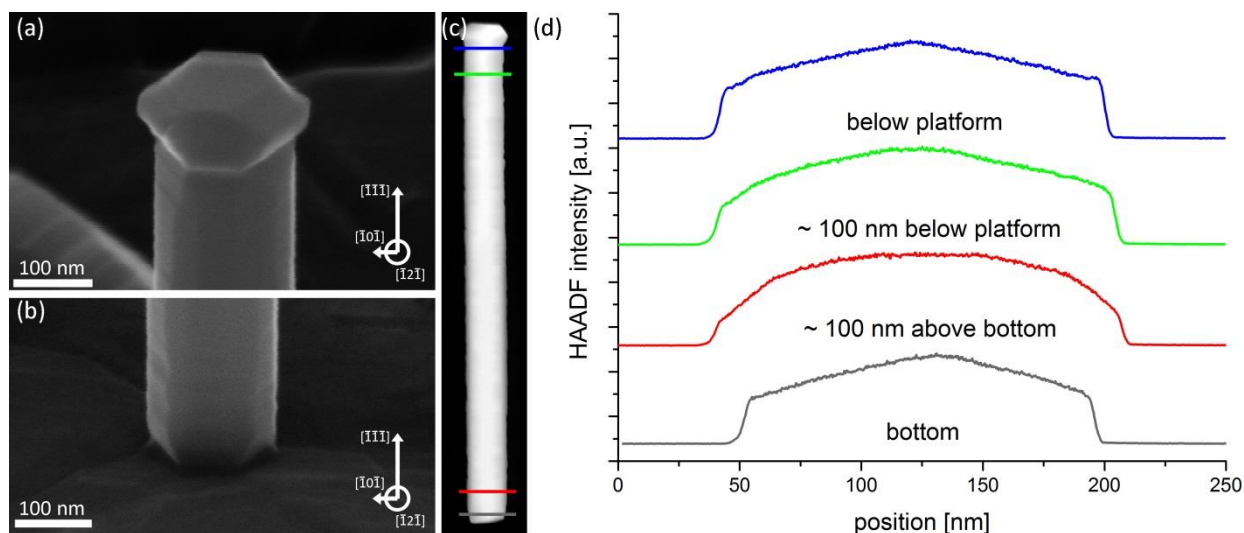


Figure S1: SEM and TEM analyses of InAs/GaSb core-shell nanowires to determine the change of the cross-sectional shape along the nanowire axis. (a), (b): SEM images from the top and the bottom. (c): STEM HAADF image of a single core-shell nanowire with colored lines indicating the position of STEM HAADF profiles shown in (d). STEM images are acquired from the  $\langle 110 \rangle$  zone axis.

## 2. Evolution of the cross-sectional shape

After the initial InAs core nanowire growth, the nanowires have a hexagonal shape. However, already 5 min of GaSb shell growth (corresponding to a nominal shell thickness of  $\sim 2$  nm) shows first evidences of a rounding of the cross-sectional shape. A further increase of the GaSb shell growth time creates clear facets of both types,  $\{110\}$  and  $\{211\}$ . In general, these facets are maintained up to thick shells of more than 40 nm. The evolution of the cross sectional shape can be followed by means of HAADF profiles plotted in Fig. S2.

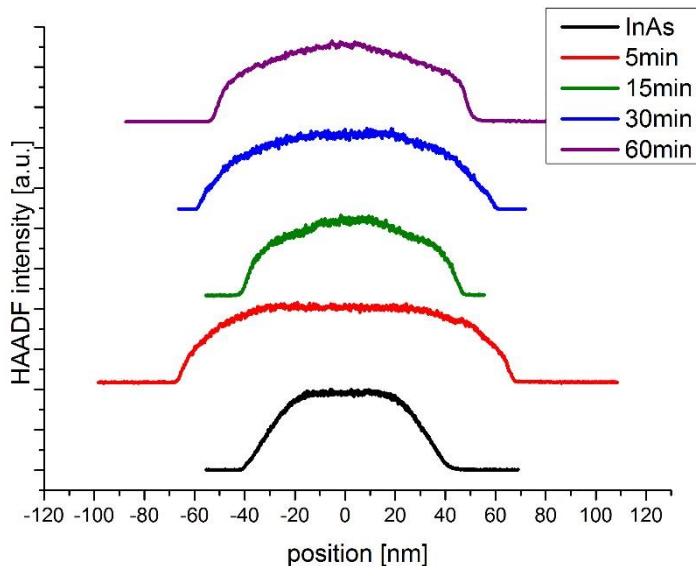


Figure S2: HAADF profiles acquired in the center of nanowires with different GaSb shell thickness (corresponding to different GaSb shell growth times). The NWs were aligned to the  $\langle 110 \rangle$  zone axis. A clear evolution from a hexagonal shape with  $\{110\}$  side facets into a dodecagonal shape can be seen. This cross sectional shape transformation starts already for shell thickness of about 2-3 nm (5min shell growth).

## 3. Comparison of the $\langle 110 \rangle$ and $\langle 211 \rangle$ zone axis for core-shell nanowire analyses

The typically used zone axis for nanowire analyses,  $\langle 110 \rangle$ , has the advantage that the crystal structure and especially potential defects such as twins and stacking faults can be identified. However, the hexagonal shape of the nanowire with  $\{110\}$  side facets results in a gradual decrease of the thickness of the nanowire towards its edges. In TEM, this gradual decrease of the thickness will prohibit an abrupt change of the contrast between the core and the shell. Similarly, performing EDX analyses from the  $\langle 110 \rangle$  zone axis creates profiles schematically depicted in Fig. S3 (upper images). Its exact shape will depend on the dimensions of core and shell and especially small shell thickness are hard to measure due to the limited spatial resolution of EDX. Thus, both techniques, TEM and EDX, have a high uncertainty regarding the evaluation of the shell thickness.

By tilting the nanowire by  $30^\circ$  around the growth axis, thus towards the  $\langle 211 \rangle$  zone axis, the crystal structure and planar defects can no longer be analyzed. However, then  $\langle 110 \rangle$  side facets are now parallel to the electron beam and therefore an abrupt change between the core and the shell can be observed. Schematically this situation is depicted in Fig. S3 (lower images). In fact, this abrupt change easily allows measuring the shell thickness and native oxide thickness. Additionally, the interface between the core and the shell can be seen from the  $\langle 211 \rangle$  zone axis with significantly less overlapping effects than from the  $\langle 110 \rangle$  zone axis.

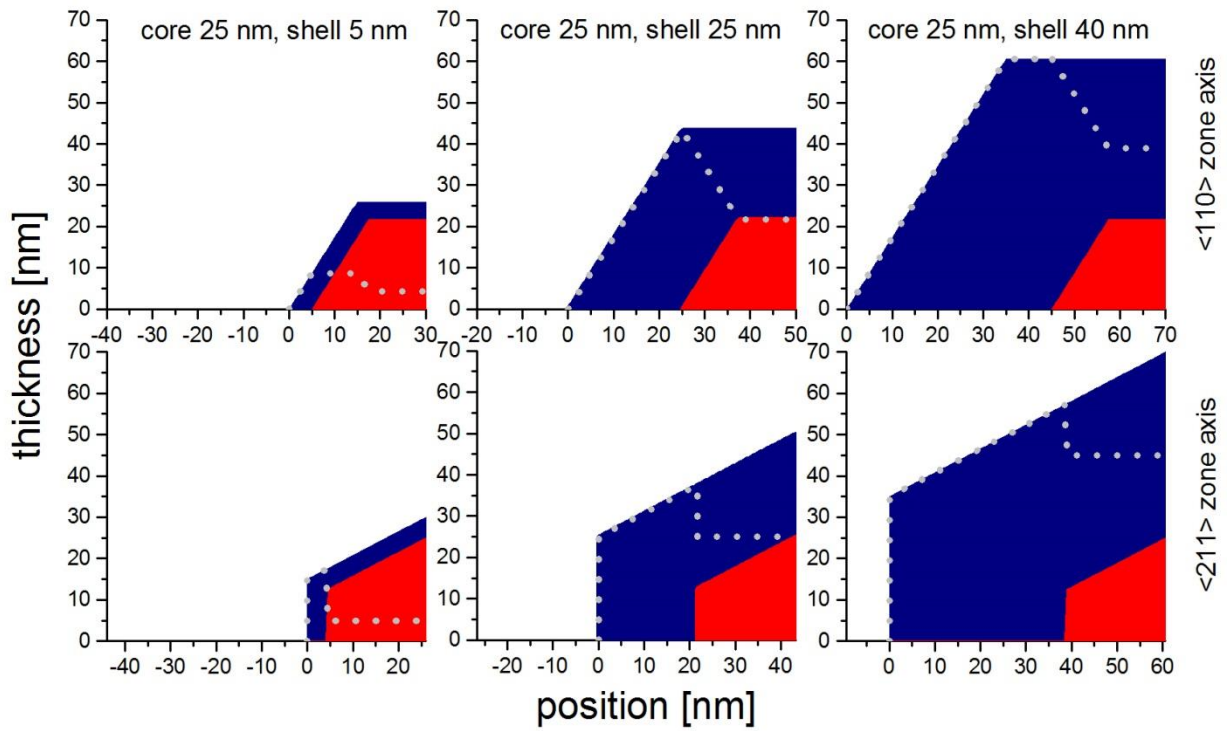


Figure S3: Schematic cross-sections of core-shell nanowires with three different shell thicknesses. The core is colored red, the shell blue. The grey dotted line represents the difference in thickness between shell and core.

#### 4. HRTEM images of the interface and evidence of misfit dislocation free growth

In the following, several HRTEM images from Fig. 6 of the manuscript are depicted in larger scale.

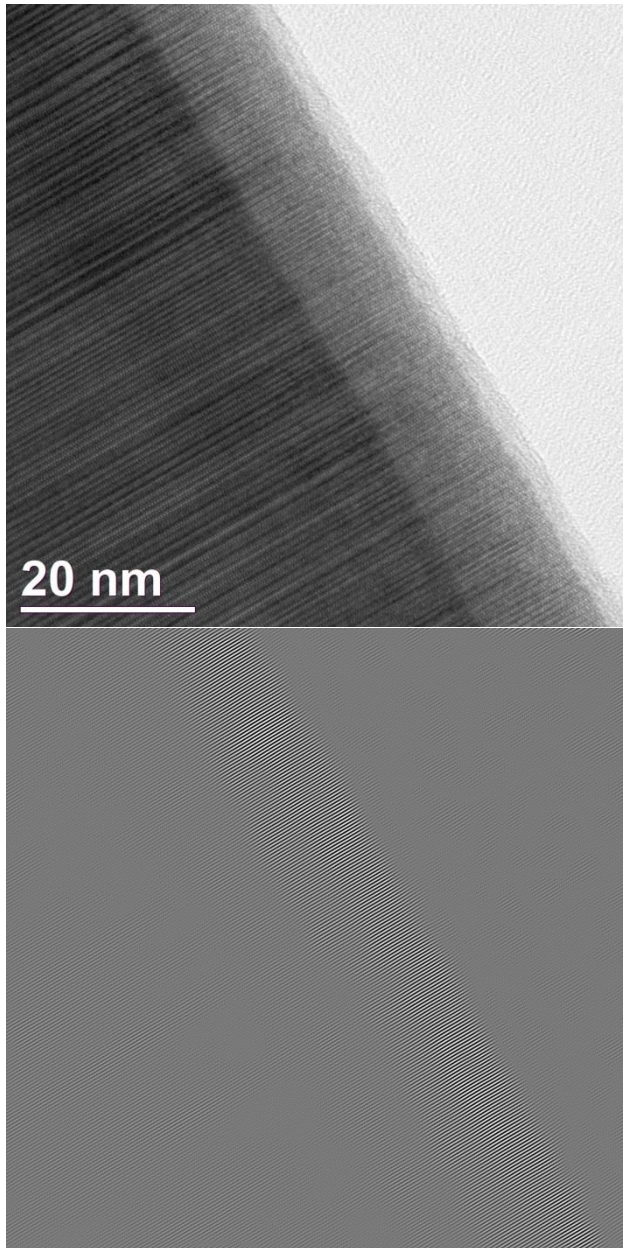
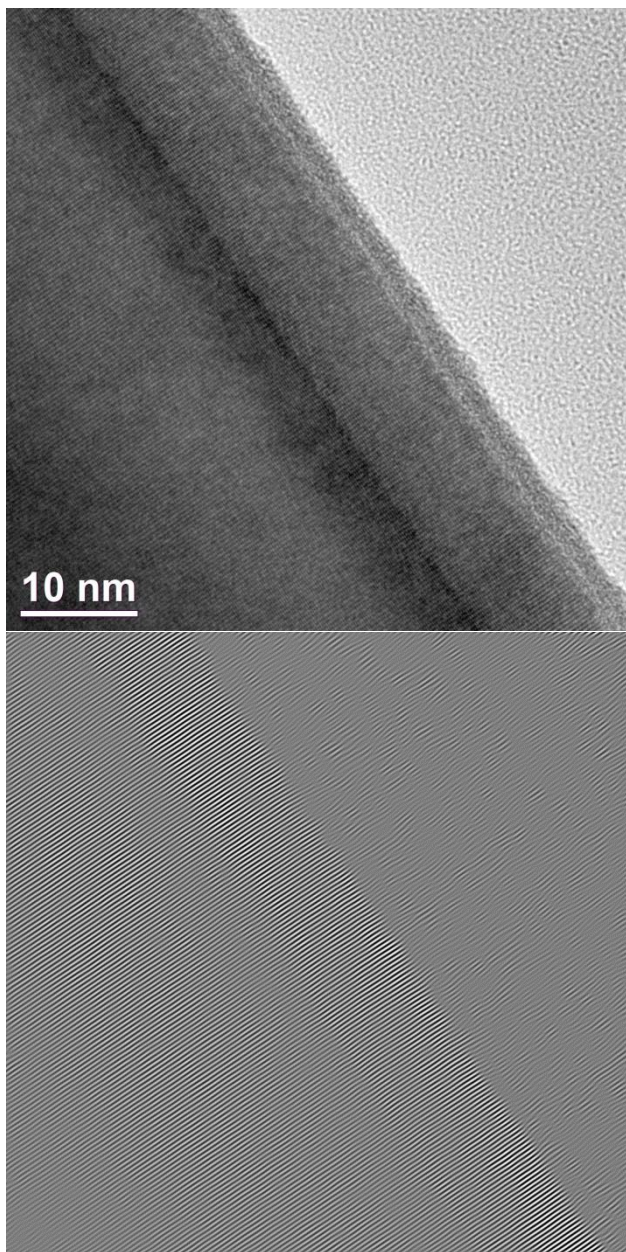
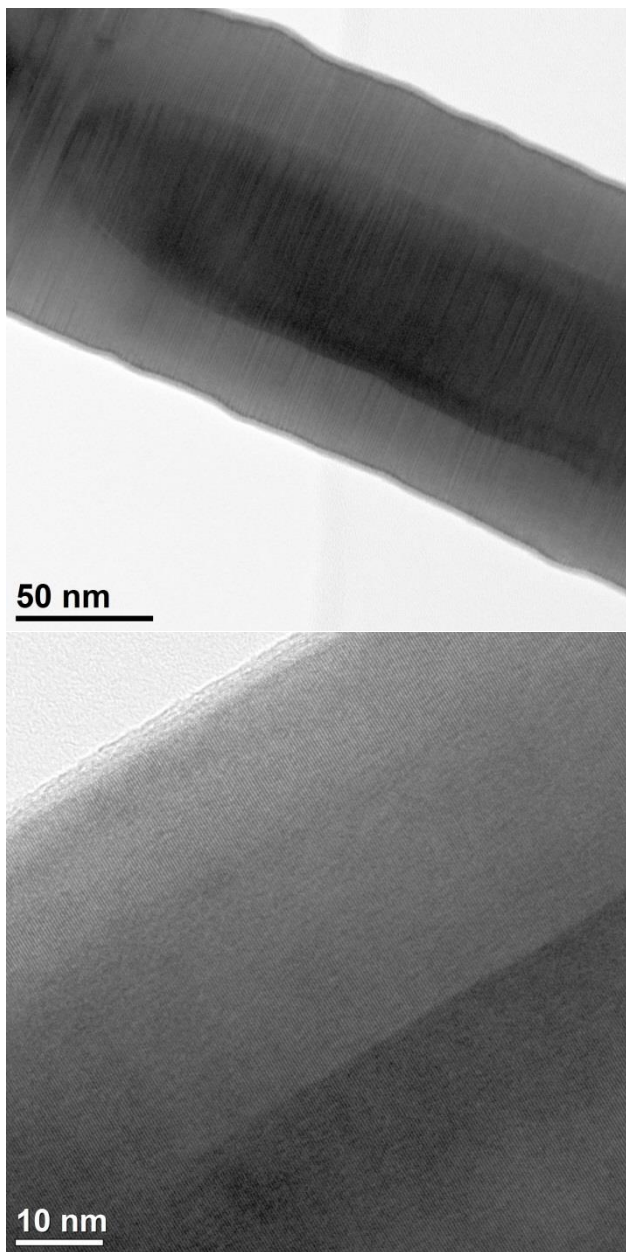


Figure S4: HRTEM and FFT-filtered image of an InAs/GaSb core-shell nanowire with  $\sim 10$  nm shell thickness. Images are taken from the  $\langle 110 \rangle$  zone axis.



*Figure S5: HRTEM and FFT-filtered image of an InAs/GaSb core-shell nanowire with ~ 10 nm shell thickness. Images are taken from the  $\langle 211 \rangle$  zone axis.*



*Figure S6: TEM and HRTEM image of an InAs/GaSb core-shell nanowire with  $\sim 40$  nm shell thickness. Images are taken from the  $\langle 110 \rangle$  zone axis.*

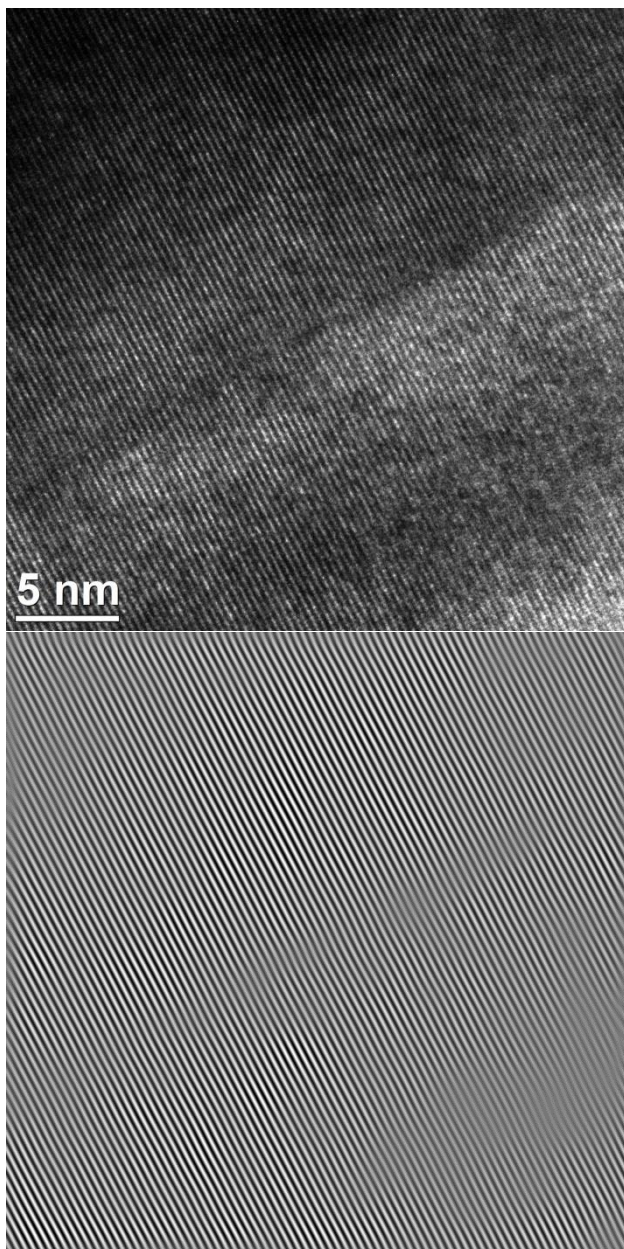


Figure S7: HRTEM and FFT-filtered image of an InAs/GaSb core-shell nanowire with  $\sim 40$  nm shell thickness. Images are taken from the  $\langle 211 \rangle$  zone axis.

## 5. Evolution of the GaSb platform

The upper region of the core-shell nanowires develops from faceted or tapered InAs into a smooth, flat GaSb platform. This platform can form additional stacking faults and twins (see main part of the manuscript and ESI section 6). Thus, the evolution of the top region is important. Fig. S8 depicts SEM and TEM micrographs of InAs/GaSb core-shell nanowires with various shell growth durations allowing following clearly the evolution of the top part. The pure InAs nanowire has a tapered top (Fig. S8a), however already 5 min of GaSb shell growth form a small, 20-30 nm wide platform (Fig. S8b and c). After about 10-15 min of shell growth, this platform has the size of the nanowire diameter, but axial growth is negligible (see Fig. S8d-f). The GaSb tends to form a uniform diameter rather than axial growth, confirming a typically low growth rate along the  $[111]_B$  direction. 30 min of shell growth, corresponding to a GaSb shell of about 11-12 nm thickness, maintains a smooth shell with a flat and uniform top facet (see Fig. S8g and h). A further increase of the shell growth time to

60 min slightly increases the diameter at the upper 100 nm, axial growth still being very low (Fig. S8i-k). Only for shell growth times longer than 60 min (shells thicker than ~25 nm), the GaSb platform with additional twins develops (Fig. S8l and m). Thus, the pronounced GaSb platform and its associated defects only develop for thick shells. Most probably the axial growth in [111]B direction is even caused by the twinning in <111>A directions.

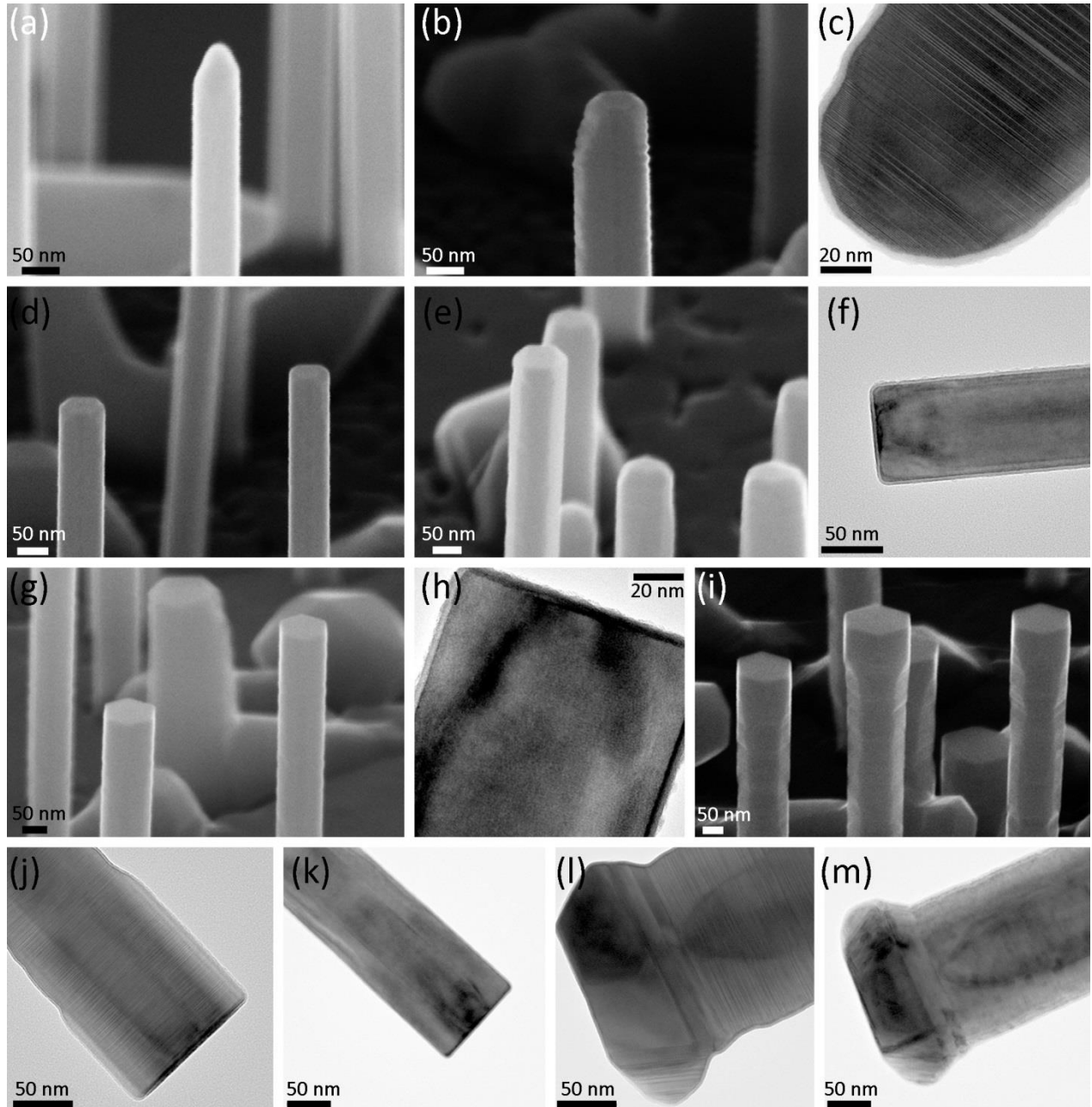


Figure S8: SEM and TEM images of the top region of InAs/GaSb core-shell nanowires with shell growth durations ranging from 0 to 90 min. (a): pure InAs nanowire, (b) and (c): 5 min shell growth, (d) 10 min shell growth, (e) and (f) 15 min shell growth, (g) and (h) 30 min shell growth, (i) – (k) 60 min shell growth, (l) and (m) 90 min shell growth. The evolution of the GaSb platform can be followed clearly. TEM images in (c), (j) and (l) are from the <110> zone axis, those in (f), (h), (k) and (m) are taken from the <211> zone axis.



## 6. Multiple-twinning induced defects in the GaSb platform

As described in the main part of the publication, the GaSb platform grown axially on top of the InAs nanowire has planar defects perpendicular to several  $\langle 111 \rangle$  directions and not only perpendicular to the nanowire growth axis. Fig. S9 depicts a HRTEM image of this region demonstrating twinning defects, here blue arrows point in  $\langle 111 \rangle_B$  directions, yellow arrows in  $\langle 111 \rangle_A$  directions. It is already described in the main part that these multiple defects can create dislocations located in the GaSb platform only; these are not caused by the lattice mismatch between the core and shell. Starting from the zinc blende region labeled A, two additional twinned lattices are formed, B and C. Of high additional interest is then the region where the two twins B and C coalesce. As can be seen from the schematic overlay, this interface (red circle) is not perfect and cannot be adjusted by additional twins or stacking faults.

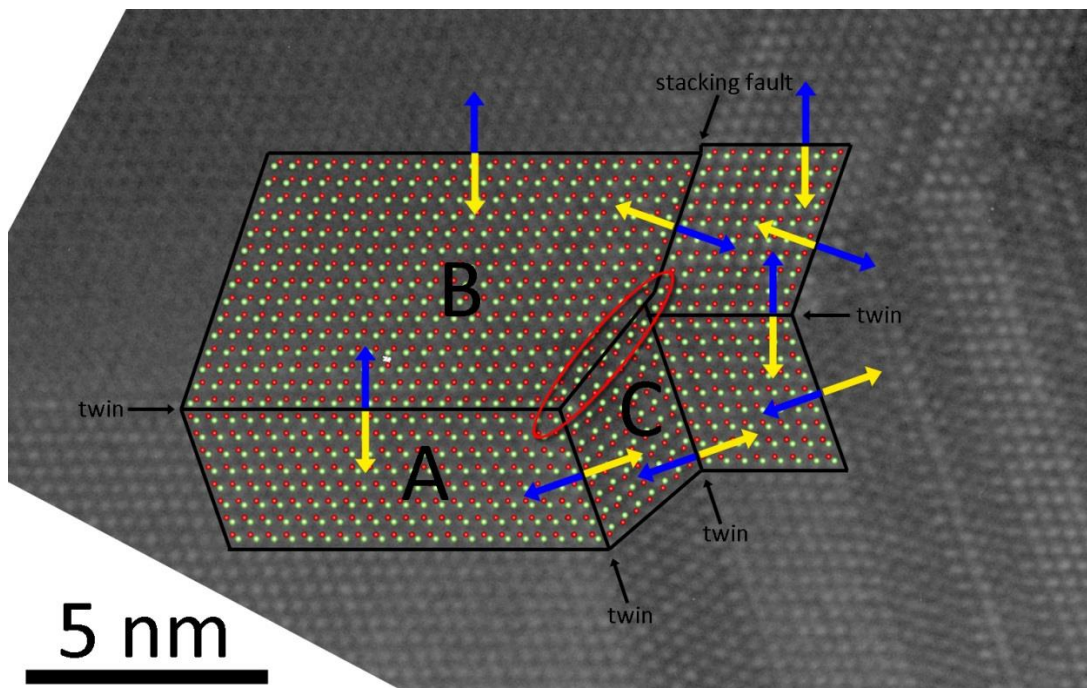


Figure S9: HRTEM image (identical to Fig. 7e) with superimposed schematic atomic arrangement, twins and stacking faults are marked by black arrows.  $\langle 111 \rangle_B$  and  $\langle 111 \rangle_A$  directions are indicated by blue and yellow arrows, respectively. The red encircled area highlights the defect region due to multiple twins.

In Fig. 10a the FFT-filtered image from Fig. 8 of the original manuscript is displayed. Red lines are used to indicate the stacking sequences in the different  $\langle 111 \rangle$  directions. It can be seen that the stacking sequence in the  $[1-1-1]_A$  direction has a high density of twins. In the  $[-111]_B$  direction only few defects can be seen, these are only stacking faults. As described above, coalescence of these twinned regions causes defects encircled in Fig. 10b. In-between these defects the stacking sequence in  $[-1-1-1]_B$  direction is twinned (see red lines in Fig. 10b). A further discussion of the structure of the defects is beyond the scope of this report.

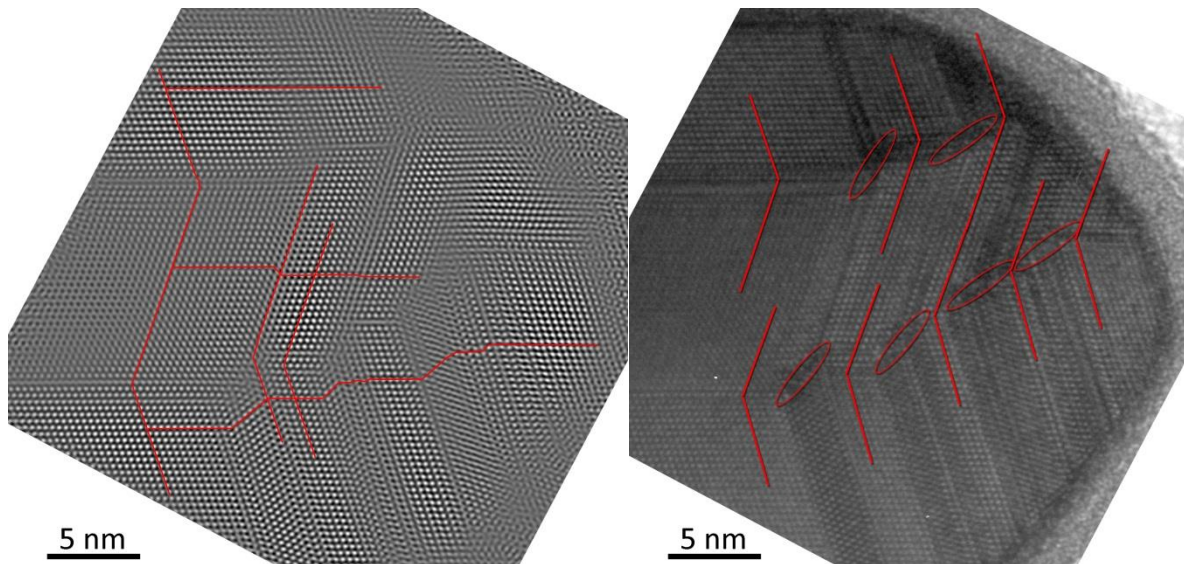


Figure S10: (a) FFT-filtered HRTEM image of the multiple-twinned region at the top of InAs/GaSb core-shell nanowires. Red lines indicate the stacking sequences in the different  $\langle 111 \rangle$  directions. (b) HRTEM image with red lines indicating the twinned ZB stacking in  $[-1-1-1]_B$  direction. Encircled areas show the defective regions due to multiple twinning.