

Structure of Single InAs Nanowires

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A method for the Au-free growth of InAs nanowires on (111) oriented Si substrates is presented which is based on a thin SiO_x layer apparently catalyzing wire growth. Structural investigations carried out by TEM and by high resolution x-ray diffraction reveal that these InAs wires contain stacking faults, i.e. regions with a wurtzite instead of a zinc-blende stacking. In order to assess the amount of the hexagonal phase, intensities from hexagonal and zinc-blende allowed x-ray reflections were measured and compared with each other.

Introduction

Semiconductor nanowires attract attention due to their potential to integrate optical functionality with mainstream Si technology. The main problem here is the fabrication of mainly III-V devices, i.e., polar semiconductor structures, on top of the unpolar Si surface. Usually the starting point are epitaxial layers, which suffer in addition to the polarity issue also from lattice mismatch values up to about 12%. The introduction of SiGe layers helps to reduce the mismatch and hence limit the dislocation densities, but a problem not easy to avoid are antiphase boundaries between regions where growth started with the group III or group V element, respectively.

Au-Free InAs Nanowire Growth on (111) Si

All these problems are greatly relieved when instead of 2D layers wires with a small diameter and a large aspect ratio are grown: with diameters around 100 nm, heights of several μm are commonly achieved. Due to the small contact region between the wires and the substrate, strain relief is easily achieved. Although it is not clear so far whether relaxation takes place purely elastically or partially plastically, no dislocations penetrating the wires are observed. Also antiphase boundaries are no big problem with nanowires.

The growth processes leading to nanowires are still under development, and the underlying growth mechanisms are not completely known. Relatively well understood are vapor-liquid-solid or vapor-solid-solid growth schemes: here, small catalytic particles, in most cases gold spheres with several 10 nm diameter, are deposited onto the substrate. Precursor gases such as trimethylgallium and arsine (just as one example) are taken up by the Au spheres, and a solid or liquid solution of Au with GaAs is formed. Once the critical concentration is reached, GaAs crystallizes, and as the energy barrier is slightly lower at the boundary from the droplet to the substrate, material starts to grow there and lift the Au-GaAs droplet up. In this way, a large number of semiconductors can be grown on various substrates. For growth on Si, however, a very unfavorable background doping with Au, which acts as a recombination centre in Si, makes the use of this growth mechanism problematic.

Recently, a different scheme was developed in collaboration between our institute and the University of Lund: it was found that instead of Au spheres, a thin SiO_x ($x \approx 1$) can

be used to “catalyze” wire growth. The details of the mechanism are still under debate: catalytic action as in the case of Au is discussed as one possibility, the formation of a growth-inhibiting SiO_2 layer with “holes” that serve as nucleation centers another [1], [2]. So far, the hard facts are as follows: using the growth scheme, wires always grow in $\langle 111 \rangle$ direction, they exhibit a hexagonal cross-section with $\{11\bar{2}\}$ side facets, and their thickness is constant from bottom to top. No “foot” region and no “catalytic particle” at the top are observed in SEM or TEM. However, TEM reveals stacking faults of the $\{111\}$ planes, where the stacking switches from an ABCABC sequence (i.e., zincblende lattice structure ZB) to ABAB (wurtzite lattice structure WZ). This indicates that the energetic difference of both lattices might be rather similar, although in bulk only ZB is stable. This could be either due to growth kinetics or be a consequence of hydrogen termination during CVD growth [3].

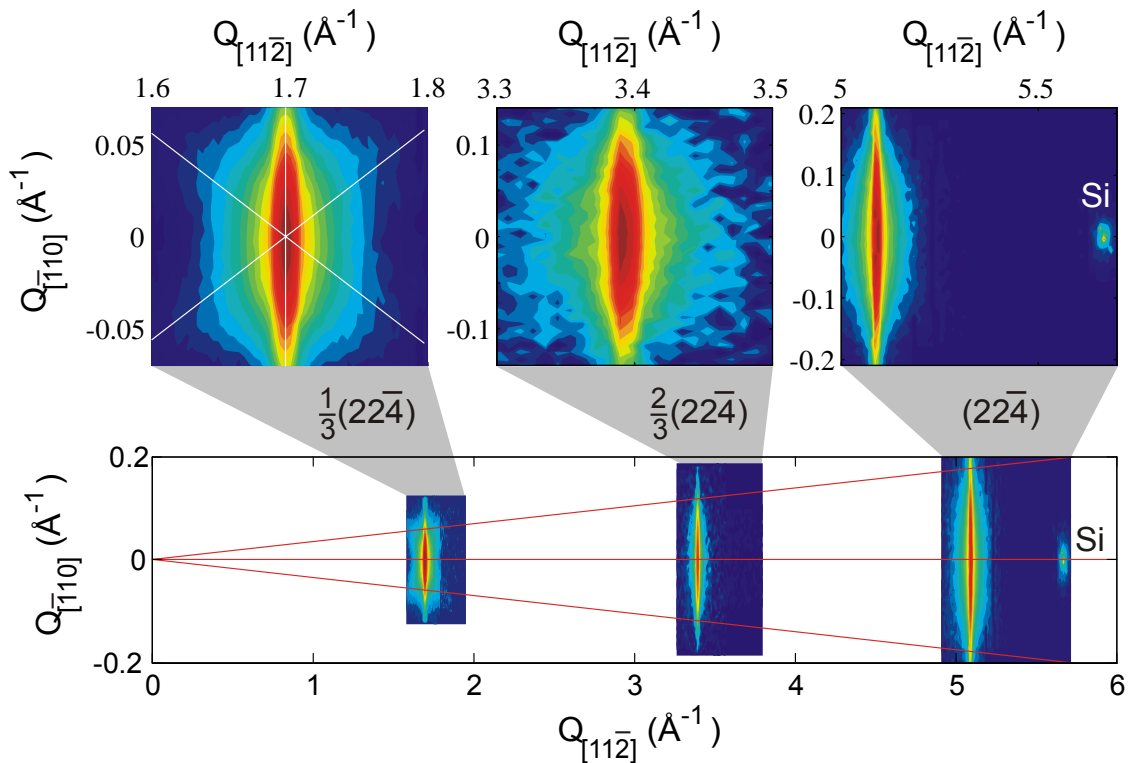


Fig. 1: Reciprocal space maps in the $[11\bar{2}]$ substrate direction. Only the $(22\bar{4})$ is allowed in the ZB substrate, the intensity around the $1/3$ and $2/3$ order reflection from the InAs wires are due to stacking faults in the wires with a local transition to WZ structure.

Structural investigations are hence required in order to understand the wire structure and the growth process. We used x-ray diffraction in order to assess the crystal quality, the crystal orientation, and the amount of stacking faults in the wires for different growth parameters. In order to assess the overall amount of WZ in the wires, measurements with a “large” beam diameter of $200\ \mu\text{m}$ were used. The intensity distribution was measured around several reciprocal lattice points to obtain the lattice parameters of InAs wires on Si(111) in the $[111]$ growth direction as well as parallel to the substrate surface. Figure 1 shows reciprocal space maps recorded in the $[11\bar{2}]$ direction of the substrate, i.e., in grazing incidence geometry. Clearly the peaks from the InAs wire material are aligned with the Si reciprocal lattice, confirming epitaxial growth. From the peak positions, the lattice parameters are determined, and it is found that InAs is com-

pletely relaxed. The $(2\bar{2}\bar{4})$ reflection is allowed in the ZB lattice of the Si substrate and the InAs wires. However, for the wires intensity is found also around the $1/3(2\bar{2}\bar{4})$ and $2/3(2\bar{2}\bar{4})$ reflections. These do not exist in ZB, but correspond to the $(10\bar{1}.0)_{\text{WZ}}$ and $(20\bar{2}.0)_{\text{WZ}}$ reflection of the WZ lattice, i.e., the intensity reflects the amount of InAs grown in the WZ structure. From the figure, a broadening of the peaks by a constant angle can be observed, which is due to a random rotation of the wires around their axis (mosaicity) with a magnitude of several tenths of a degree, depending on the growth conditions. For the lowest order reflection, streaks perpendicular to the wire side facets are observed due to the hexagonal wire shape. For the higher order reflections, these streaks are smeared due to the peak broadening.

Discrimination between Cubic and Hexagonal Phase

In order to quantify the WZ amount, we integrated the intensity of the three in-plane reflections as shown in Fig. 1 for each sample. Knowing the structure factors for the reflections as well as the amount of illuminated wires (which changes due to the changing Bragg angle from reflection to reflection), we can calculate the intensity decay as a function of peak order. This is plotted in Fig. 2 as dashed line. The experimental data are plotted as symbols, the intensities are normalized to the $(10\bar{1}.0)_{\text{WZ}}$ reflection. The excess intensity for the $(30\bar{3}.0)_{\text{WZ}}$, which is equivalent to the cubic $(2\bar{2}\bar{4})$ reflection, is due to the ZB part of the wires. Evaluating these data reveals that only 10 – 20% of the wire volume grows in the WZ lattice.

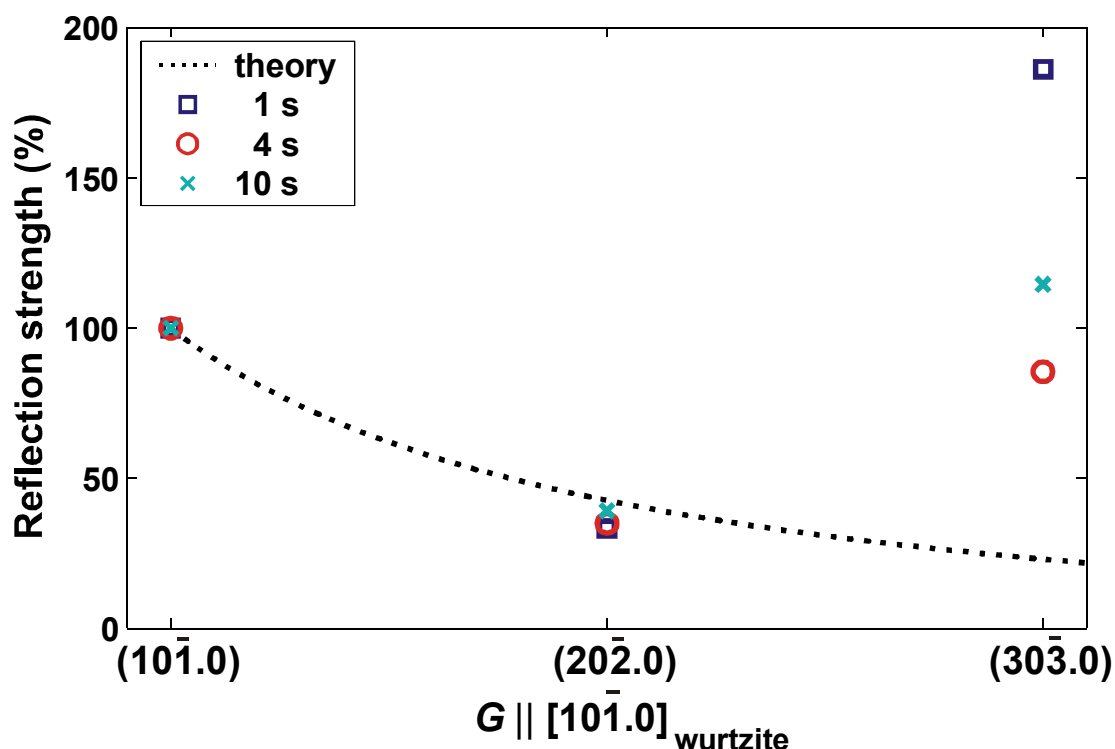


Fig. 2: Intensity from InAs wires as a function of reflection. Dashed line shows the theoretical behavior for pure WZ lattice. The experimental points show the measured intensity normalized to the $(10\bar{1}.0)_{\text{WZ}}$ reflection. The excess intensity for the $(30\bar{3}.0)_{\text{WZ}}$ is due to the ZB part of the wires.

Summary

From the data, no information is obtained concerning the length of the WZ and ZB segments in the wires. If the energies of both configurations are almost equal, longer WZ segments can be expected, whereas shorter segments indicate that ZB is still the more stable lattice, and WZ is only introduced as a defect. Recent measurements using coherent diffraction, where the interference between the radiation scattered from different WZ segments of one and the same wire are observed, rather hint on the latter, but the data analysis is not yet conclusive enough.

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References

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