



	Experiment title: Strain accommodation at the interface between homo-and hetero epitaxial InP(InAs) nanorods grown onto <111>B InP(GaAs) substrate	Experiment number: SI-1470
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Report: The aim of the experiment was to investigate the the nanorod (NR)- substrate interface of semiconductor nanorods by surface sensitive x-ray diffraction technique. For this purpose we have investigated homoepitaxial InP NR's VLS-grown onto <111>B InP and heteroepitaxial InAs NR onto <111>B GaAs using x-ray grazing-incidence diffraction at ID10B at energy of 8 keV. The beam size was reduced to 0,1 micron vertically and 1 microm horizontally. First we measured long 2:1 in-plane scans ($30^\circ < 2\Theta < 110^\circ$) at an incidence angle α_i smaller or larger then critical angle of total external reflection, α_c , in order to analyse whether the rod structure is wurzite or zinc-blende type. In case of InAs/GaAs[111B] (see Fig.1) grown from Au seed [1] we found two strong Bragg reflections corresponding to (2-20) and (4-40) reflection of zinc-blende but only small contribution of wurzite at (21-30) reflection. At the same time we found additional peaks corresponding to cubic Au clusters with 1-2% increase in the lattice parameter caused by alloying with Indium. The wurzite contribution was missing at the InP homoepitaxial samples (not shown) which were VLS grown without Au seed [2]. Next we screened the α_i dependence in the vicinity of (2-20) and (4-40) reflections. High resolution x-ray diffraction scans through the (4-40) reflection of InP nanorods grown homoepitaxial onto InP [111B] are shown in Fig.2. From peak width one can clearly distinguish between the InP substrate (sharp peak) and the InP NR. The mismatch is -0,3% independent from incidence angle α_i . Therefore the smaller lattice parameter is associated to the NR, probably caused by a shrinking of next neighbor distances close to the NR surface Considering the average diameter of InP NR of 27nm and assuming all next neighbor distances except the first atomic layer below the surface have the same atomic distances as InP in bulk the surface lattice parameter is shrinked by 6,5% copared to the bulk value to reproduce the experimental finding.

The same measurements have been performed at heteroepitaxial InAs NRs grwon onto GaAs[111B]. As shown in Fig.3 at the (4-40) reflection two major peaks are visible. The low angle peak belongs to InAs the peak at higher angles is a measure for GaAs. The peak in between corresponds to the Au:In alloy. The α_i dependence provides additional information. As long as $\alpha_i < \alpha_c$ the interaction of the incident beam with the substrate surface is small and the diffracted intensity mainly is a probe of the NR. Increasing to $\alpha_i \geq \alpha_c$ the beam will penetrate into the substrate and probes the structure at the interface in addition. As seen in Fig.3 there is a shoulder in intensity at the high angle side of InAs. It changes in intensity by one order of magnitude straight after increasing the incidence angle to $\alpha_i > \alpha_c$. The same is found at the background of GaAs. These additional features must be associated with the InAs to GaAs interface. Fig.4 shows the α_i -dependence at several angular positions taken from Fig.3. The intensity of InAs NR varies as function of the illuminated area. The GaAs peak intensity is large at negative α_i , here we scatter from the backside of substrate. Its intensity drops for increasing α_i but increases again at $\alpha_i \geq \alpha_c$. All other features show a steep increase in intensity straight at $\alpha_i = \alpha_c$. In order to evaluate the data we have simulated the main diffraction peaks of InAs and GaAs by appropriate Voigt functions. From FWHM of InAs peak we evaluated an average

diameter of InAs NR of about 60nm which is in accordance with SEM inspection. The remaining features at the high angle side of InAs could not be simulated by a single extra peak but it required a set of peaks with slightly different lattice parameter. Here we used the same peak widths as extracted from InAs NR. In addition we have found similar deformations of the InAs Bragg peak at out-of plane reflections (not shown here). Considering a linear relation between the lattice parameter and In-concentration in $\text{In}_x\text{Ga}_{1-x}\text{As}$ solid solution we can associate the measured variation of lattice parameters by a variation of Ga concentration between 6% and 22%.

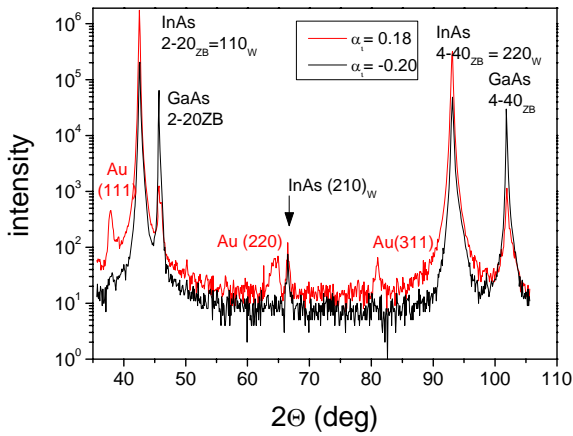


Figure 1 In-plane scans at InAs/GaAs [111B] NR structure grown by MOVPE taken at two different α_i .

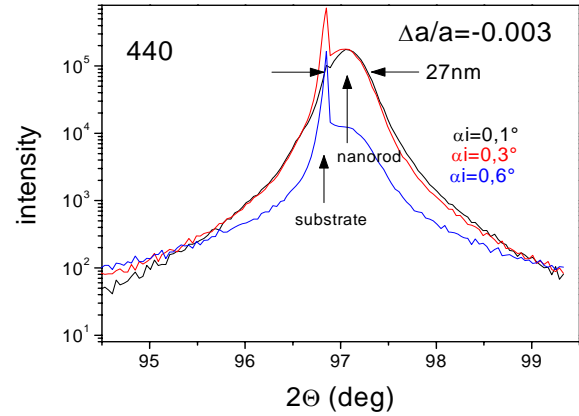


Figure 2: High-resolution in-plane scans through 4-40 Reflection of InP NR grown homoepitaxially onto InP[111B] substrate

Our results can be interpreted by the appearance of a wetting layer on top of GaAs substrate which contains a certain amount of Indium. Out of this wetting layer several InGaAs nuclei of NR start growing at positions of Au droplets via VLS-growth mode. Due to the only presence of In and As from gas phase the growth of NR will be stopped and the growth of pure InAs NRs will continue solely.

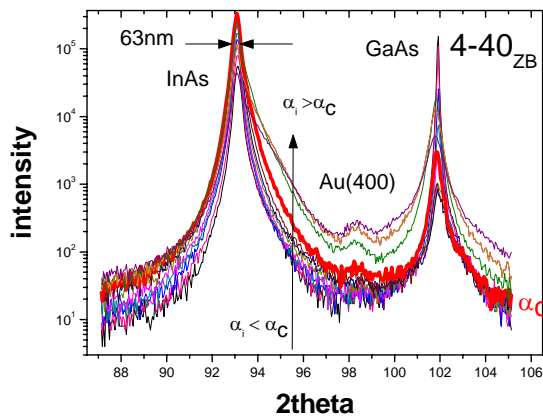


Figure 3 High resolution scan through the (4-40) reflection of heteroepitaxial InAs NRs grown on GaAs [111B]

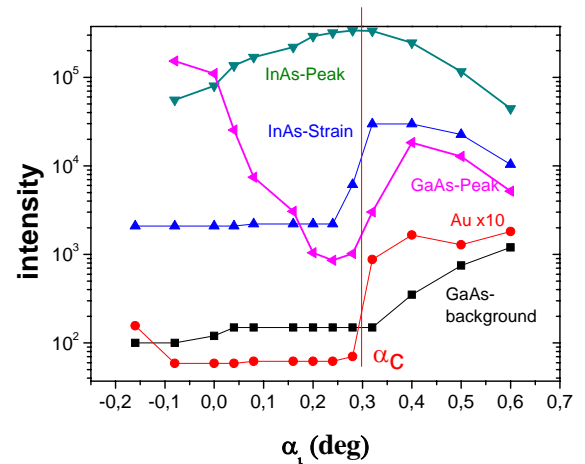


Figure 4: α_i dependence of structure parameters taken from Fig.3

References

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