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## **Report:**

We have systematically studied a series of InAs/InAsP core-shell wire structures. The samples have been grown by chemical vapor deposition at the University of Lund, Sweden [1,2] on Si(111) substrates. Wire nucleation is achieved by an allyl-alcohol layer on the Si surface, which partially decomposes in the CVD chamber [2]. The wire core consists of pure InAs with a nominal thickness of 100 nm and a length of about 2  $\mu$ m. Subsequently the wires are covered by a shell of InP: pure InP is deposited, and the deposition time varied in order to produce a different shell thickness. Additionally, samples with a shell of InAsP, i.e., with a different mismatch of the shell to the wire core, have been investigated.

X-ray diffraction (XRD) experiemnts in coplanar diffraction geometry and grazing incidence diffraction (GID) confirm a good epitaxial relationship between wires and substrate. The main question addressed here is the shell thickness and composition, as well as the strain state of wire and shell. To obtain a low-noise signal from the wires, reciprocal space maps have been recorded in GID geometry around several in-plane reflections, reducing the signal from the substrate. The latter can be almost completely suppressed taking advantage of the fact that the wires partially grow in wurtzite lattice structure, while the other part of the wires and the substrate (together with any possible 2D layer on top of the substrate) has zincblende lattice structure: selecting in-plane reflections which are allowed only for the wurtzite, the substrate scattering is virtually absent. Figure 1 shows as colormaps reciprocal space maps for two samples with high and low InP content in the shell.



Fig. 1: Reciprocal space maps of two InAs-core/InAsP-shell wire structures with about 100 nm core diameter and 50 nm shell thickness. The color map shows experiemtnal data, black contour lines are simulations based on FEM calculations and kinematical scattering theory. For the sample shown in the left panel, a good fit is obtained for a InP content of 28%. For the sample in the right panel, no good correspndence could be achieved: The simulation shown, where the peak positions roughly fit, but the peak shape does not, is based on a InP content of 44%. Since the model takes into account only a pseudomorphic relationship between core and shell, this indicates that for this InP content plastic relaxation is already important.

In previous experimetns (cf. reports to Si-1395 and Si-1245) it was found that the scattering can be well simulated using kinematical scattering theory. The contour lines in Fig. 1 show such simulations: an FEM model of the core-shell wires was used to calculate the strain distribution in core and shell for different shell mismatch and shell thickness values. These values were varied until a good correspondence between experiment and simulation was achieved. Obviously, for the low InP content, the correspondence is very good, while for the high InP content no good fit could be obtained for any set of parameters, indicating that for this sample the model assuming a pseudomorphic relationship between core and shell is not valid any more. This means that for the high InP content plastic relaxation processes play already a role. While we could successfully establish how to detect the presence of plastic relaxation, the sample series is not sufficient to allow for a systematic study of the onset of plastic relaxation and a corresponding "critical thickness" or "critical strain".

## **References**

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