ESRF	**Experiment title:** Strong tensile strain in the extremely thin core of individual GaAs/InxGa1-xAs core/shell nanowires as a function of the shell thickness and composition	**Experiment number**: HC-3196
Beamline:	**Date of experiment**: from: 20.10.2017 to: 23.10.2017	**Date of report**: 02.03.2020
Shifts:	**Local contact(s)**: Tobias Schülli	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Genziana Bussone*, DESY Photon Science, Notkestr. 85, 22607 Hamburg, Germany

Raphael Grifone*, DESY Photon Science, Notkestr. 85, 22607 Hamburg, Germany

Emmanouil Dimakis, Helmholz-Zentrum Dresden Rossendorf (HZDR) Institute of Ion Beam Physics and Materials Research, 01314 Dresden, Germany

Jörg Grenzer*, Helmholz-Zentrum Dresden Rossendorf (HZDR) Institute of Ion Beam Physics and Materials Research, 01314 Dresden, Germany

Report:

Aim of the experiment X-ray diffraction (XRD) with a coherent nano-focused beam was used to study quantitatively the radial distribution of misfit strain (in-plane and out-of-plane) at different positions along the growth axis of individual core/shell nanowires. This new knowledge will contribute to the understanding about relaxation mechanisms in highly lattice mismatched core/shell NWs, with the final goal of tailoring the strain-dependent properties at the nano-scale. The possibility for monolithic integration of core/shell in Si-CMOS platforms adds to the technological significance of our work.

Sample description The samples of GaAs/$In_xGa_{1-x}As$ core/shell NWs were grown by molecular beam epitaxy (MBE) on Si(111) substrates. Structural parameters, such as In concentration and shell thickness were tuned by controlling the growth temperature, the growth duration and the In-flux. A sample with core diameter of 20 – 25 nm, nominal In-concentration in the shell of x=0.16 and shell thickness of 40 nm was characterized in this study. A preparation of the sample using SEM and FIB was performed before the experiment at the DESY NanoLab in Hamburg. Here L-shaped markers (tens of micron large) were milled on the sample surface with a focused-ion-beam, in order to mark the areas where isolated nanowires (within a radius of 6 to 7 microns) could be identified on the sample.

Experimental technique and data collected The experiment was carried out at beamline ID01 at a X-ray energy of 10keV. The X-ray beam was focused down to ~300nm (H) by ~150nm (V) using a Fresnel Zone

Plate. An optical microscope, in combination with K-Map scanning X-ray microscopy configuration was used to identify the markers on the sample surface and the pre-selected nanowires. The following reflections have been measured:

(I) The out-of-plane symmetric reflection (111) of three individual nanowires at their original position on the growth substrate was investigated. Here, for one of the nanowires, the same reflection was collected at different positions along the growth axis.

(II) The out-of-plane asymmetric (422) and (331) reflections were collected for one of the same nanowires described above.

(III) The in-plane (20-2) reflection was measured for two laying nanowires after dispersion on a clean Si substrate. Here, for one of the nanowires, the same reflection was collected at different positions along the growth axis.

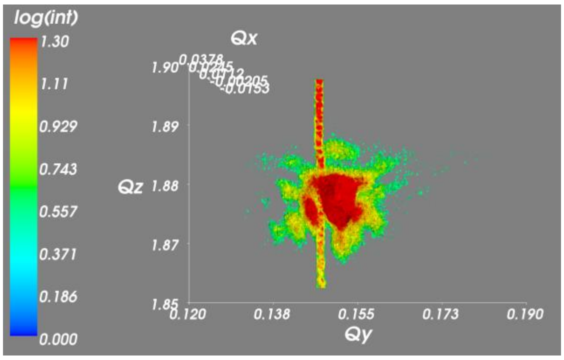

Figure 1 Preliminary calculation of a three dimensional reciprocal space map of reflection (111) collected for an individual nanowire at its original position on the growth substrate.

<u>Data treatment</u> Three-dimensional reciprocal space maps (RSM) have been calculated from the sets of MaxiPix detector images for each Bragg reflection collected. The two-dimensional detector images have been converted from angular to reciprocal space as a first step of the data extraction. The components of the wave vector transfer q_r and $q_{t(x,y)}$, respectively, are defined as parallel and perpendicular to the normal of the family of planes under investigation, where the x and y components are separated by a 90° angle. Figure 1 shows the preliminary calculation of a three dimensional RSM for an individual nanowire. Here the presence of thickness oscillation fringes can be observed.

<u>Expected results</u>

Here the presence of hydrostatic strain in individual core/shell nanowires with a shell thickness of 40nm is under investigation. The data collected at different axial positions along the same nanowire will be combined with recent EDX investigation of material concentration on similar structures, with the goal to look for a correlation. In addition, FEM simulations are currently being performed with Comsol Multiphysics with the objective to simulate the measured diffraction patterns. The characterization of the out-of-plane and in-plane strain distribution along the growth axis of individual nanowires will complement the study recently published in the following manuscript *Balaghi L., Bussone G., et al., Widely tunable GaAs bandgap via strain engineering in core/shell nanowires with large lattice mismatch, Nat. Comms. 10 (2793), 2019*.

In addition, the experiment performed at ID01 is supporting the preparation of a beamline instrumentation manuscript titled “A flexible experimental configuration for X-ray diffraction on individual nanostructures at beamline P08-DESY”. The same nanowire was indeed characterized in the two systems: here the improved data quality of beamline ID01 will strengthen the interpretation of the first nano-focused XRD experiment performed at beamline P08 at the PETRA III synchrotron.