ESRF	**Experiment title:** Internal parameter of GaP nanowires in the wurtzite phase	**Experiment number:** HC615
Beamline: ID01	**Date of experiment:** from: 26 April 2013 to: 29 April 2013	**Date of report:** 30 August 2013
Shifts: 9	**Local contact(s):** Jan Hilhorst	*Received at ESRF:*

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Report:

From the results obtained during this beamtime an article entitled:
"Unit cell structure of the GaP wurtzite phase" by
Dominik Kriegner, Simone Assali, Abderrezak Belabbes, Tanja Etzelstorfer, Václav Holý, Tobias Schülli, Friedhelm Bechstedt, Erik PAM Bakkers, Günther Bauer, and Julian Stangl
was prepared and recently accepted in *Physical Review B*

Abstract
We present structural characterization of the wurtzite crystal structure of GaP nanowires, which were recently shown to have a direct electronic band gap. The structural parameters of the wurtzite phase do consist of two lattice parameters and one internal degree of freedom, determining the Ga-P bond length along c-direction. Using density functional theory calculations, we study the influence of the internal degree of freedom on the band structure. By synchrotron x-ray diffraction studies near the Ga-K edge we determine the lattice parameters $a = 3.8419$ Å and $c = 6.3353$ Å as well as the internal degree of freedom $u = 0.37385$ with high accuracy. We find that different Ga-P bond lengths are not equal in contrast to the case in the zincblende bulk phase. As a result, a spontaneous polarization is predicted for wurtzite GaP.

In the article the lattice parameters and the internal structure of the GaP unit cell were determined from the Bragg peak positions as well as intensities of a series of measured Bragg peaks. These Bragg peaks are located along crystal truncation rods of type $(h0\bar{h}.\bar{l})$ with $h = 1, 2$ as illustrated in Fig. 1 and the 3D intensity distribution around such Bragg peaks was measured. Using kinematical theory the peak intensity was simulated and from the comparison with the experiment the internal degree of freedom of the wurtzite phase was determined. The results were compared with density functional theory calculations, which also show the influence of the internal parameter onto the direct band gap of wurtzite GaP.

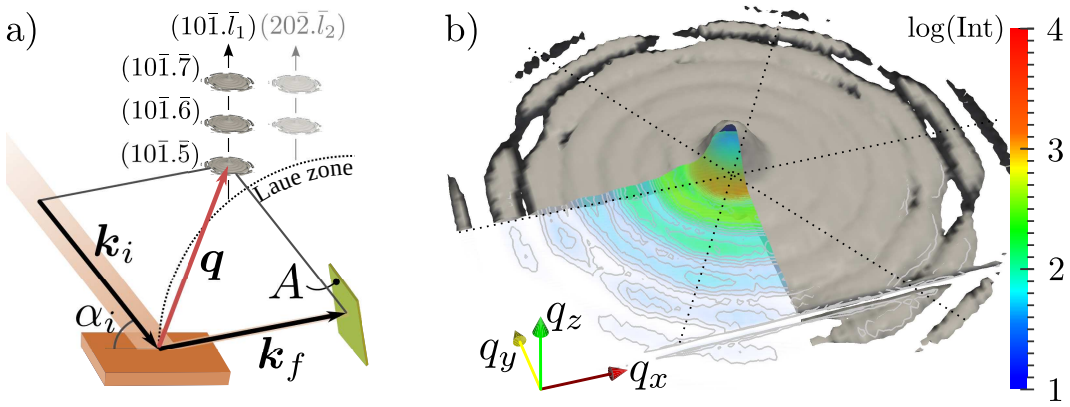

Figure 1: *Panel a) shows a sketch of the diffraction setup with the primary and diffracted wave vectors $\vec{k}_{i,f}$ as well as their difference the momentum transfer $\vec{q}$. The diffraction positions of some $(h0\bar{h}.\bar{l})$ Bragg positions along [000.1] crystal truncation rods are illustrated. In panel b) a three dimensional contour plot of the measured intensity pattern of the $(10\bar{1}.\bar{5})$ WZ Bragg reflection is shown. The contour plot is cut open to show the intensity variation inside as a semitransparent color plot. Dotted lines indicate the facet streaks due to the hexagonal cross section of the nanowires.*