	Experiment title: **Local structure of Ga and As in InGaAsN quantum wells by DAFS**	**Experiment number**: HS 2020
Beamline: BM 02	**Date of experiment**: From: 03/04/03 to: 08/04/03	**Date of report**: 24/08/04
Shifts: 15	**Local contact(s)**: Dr. H. Renevier	*Received at ESRF:*

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Report:

The aim of this experiment was to study the local structure of InGaAsN/GaAs single quantum wells (QWs) and the effects of hydrogenation on the interatomic distances using Diffraction Anomalous Fine Structure at the Ga K-edge, in order to clarify the structural origin of the anomalous electronic properties of these alloys. The use of a high-brilliance SR source was mandatory in order to perform these measurements on 6 nm epilayers. InGaAsN alloys are important from a technological viewpoint because they can be grown lattice matched to GaAs varying the emission wavelength gap in the range 1.3–1.55 μm; since these two limit wavelengths correspond to the minima for attenuation of the signal into silica optical fibers, these materials can be used for the construction of laser diodes coupled to the fibers. These devices have improved temperature characteristics compared to InGaAsP/InP diodes. From the viewpoint of fundamental physics, InGaAsN has intriguing physical properties that derive from the large mismatch between the dimensions of the N atom and the other constituents. The most obvious anomaly is that the optical band gap actually decreases, rather than increasing, with N concentration. Physical properties have been observed to be strongly non-linear with the N concentration and a dependence on atomic ordering of the constituent atoms has been predicted [1] and observed [2,3,4].

This DAFS experiment, recently conducted, was successful thanks to the advanced facilities present at ESRF: good quality data was obtained, despite the very low thickness of the

InGaAsN layer. We measured the fine structure of the diffracted intensity beyond the Ga K-edge at the weak (006) reflection; the Bragg peak maximum intensity was recorded as a function of the energy. The choice of a weak reflection guaranteed a strong anomalous effect (Fig. 2), and the use of a crystal analyzer was necessary in order to separate the diffraction peak from the Kα and Kβ fluorescence ones (Fig. 1); such a set up was exploited for the first time at the BM02 beam line of the ESRF during our experiment. Beam-time was not enough to measure also the As K-edge on a sample series, due to multiple diffraction distortions.

Data analysis was performed by using the DPU code to fit the smooth part of the DAFS spectrum, the Autobk code for background subtraction, the FEFF8 code for modeling the theoretical phases and, finally, the Feffit code for fitting the experimental data; background subtracted spectra and fits on the first shell Fourier filter are reported, respectively, on panel a) and b) of Fig. 3 for the three measured QWs (InGaAs, InGaAsN, hydrogenated InGaAsN).
The good quality of data permitted to find out that in the hydrogenated QW the Ga-As bond length is greater than the value predicted by the classic theory of elasticity in semiconductors (Fig. 4). This result, which is in agreement with results on the In-As bond lengths extracted by EXAFS at the In K-edge, is explained in the frame of the local effects of a particular N-H complex [5] whose formation has been observed to bring about a relaxation of the unit cell of the alloy [6]. On the basis of these results we are preparing a paper, which is almost ready for submission to the Physical Review B.

References:

[1] Kim and Zunger, Phys. Rev. Lett. 86, 2609 (2001)
[2] G. Ciatto et al., Phys. Rev. B 68, 161201 R (2003)
[3] V. Lordi et al., Phys. Rev. Lett. 90, 145505 (2003)
[4] G. Ciatto and F. Boscherini, J. Phys.: Condens. Matter 16, S3141 (2004)
[5] A. Janotti et al., Phys. Rev. Lett. 89, 086403 (2002)
[6] A. Polimeni et al., Phys. Rev. B 68, 085204 (2003)

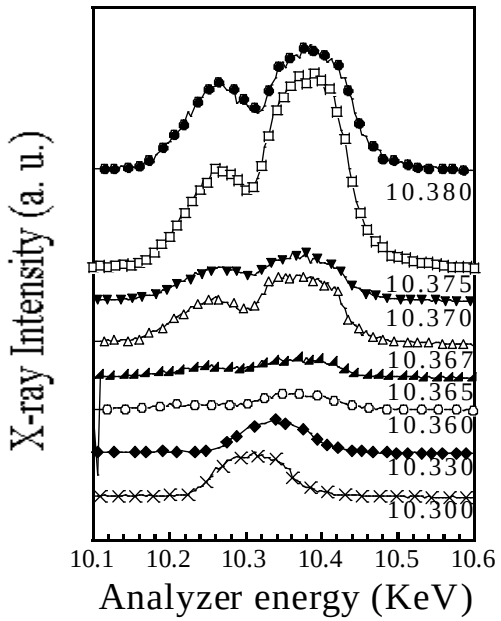

Fig. 1: Energy scans perfomed with the analyzer for different values of the incident beam energy

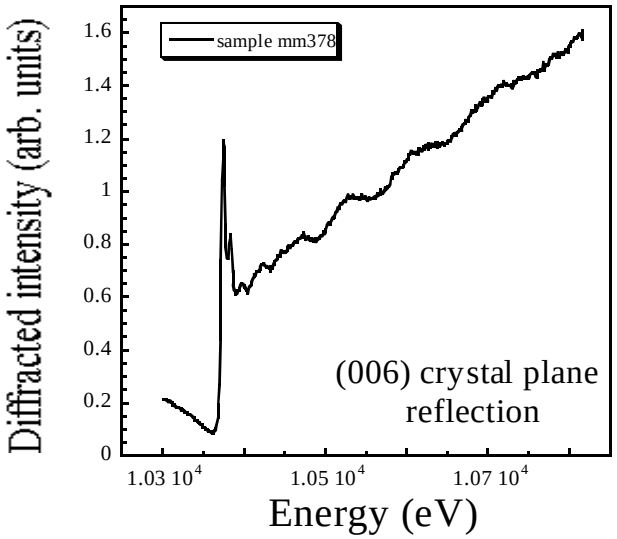

Fig. 2: Normalized diffracted intensity at the (006) crystal plane reflection around the Ga K-edge

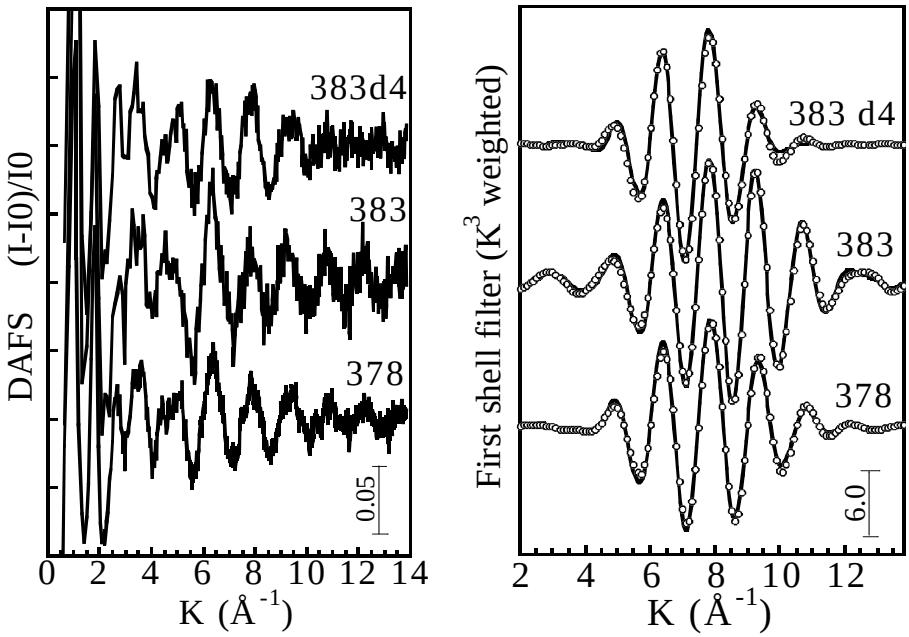

Fig. 3: a) Background subtracted DAFS spectra for the three investigated QWs; b) Fits on the first shell filter (k^3 weighted): continuous line = data, dots = fits.

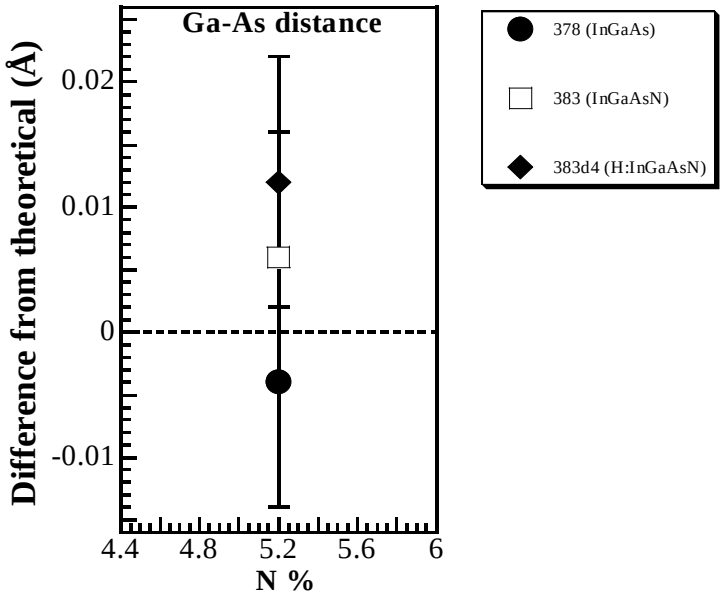

Fig. 4: Difference between experimental and theoretical determination of the Ga-As distances; circles = InGaAs, squares = InGaAsN, diamonds = hydrogenated InGaAsN. Errors = 1σ.