	Experiment title: ÉTUDE EXAFS DE FILS ET BOITES QUANTIQUES DE SEMICONDUCTEUR III-V. XAFS STUDY OF III-V SEMICONDUCTORS QUANTUM WIRES AND QUANTUM DOTS	Experiment number:
Beamline:	**Date of experiment**: from: 18/06/03 to: 21/06/03	**Date of report**: 15/10/04
Shifts:	**Local contact(s)**: Dr. X. Biquard	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Dr. Hubert RENEVIER*

Dr. Maria Grazia PROIETTI*

Dr. Jorge M. GARCIA

Dr. Michel GENDRY

Dr. Jean Michel GERARD

Dr. Luisa GONZALEZ

Dr. Cristelle MONAT

Report:

Preliminary measurements on a serie of GaN/AlN Quantum Dots (QDs) samples, were carried out at the CRG beamline FAME (BM30) (ref. n. 3002-636). EXAFS spectra were recorded in fluorescence mode at the Ga K-edge, with the polarization vector perpendicular to the surface, that is to the growth plane, along the [001] direction.

The samples consist of GaN/AlN QDs grown onto SiC substrates by MBE in the Modified Stransky-Kranstanov regime [1]. The QDs layer is capped by an AlN spacer layer. The sequence GaN QDs/AlN spacer is repeated 3, 10 and 78 times, as shown in Table I. The spacer layer thickness is about 7nm for samples s1582, s1580 and s1581 and 11nm for sample E242. The equivalent GaN thickness is 6ML for the first three samples and 4ML for the last one.

Depending on the AlN spacer, a strain driven correlation mechanism between each QDs layer and the layer underneath, can take place. In that case the QDs tend to pile up getting larger and more homogeneous in size. Samples S1580 and S1581 are supposed to be correlated whereas sample E242 is not.

The EXAFS analysis has been carried out by using the FEFF8 code, to generate theoretical phases and amplitudes, taking into account beam polarization. The Artemis package was used to fit theoretical signals to the experimental data. As an example, we show the best fit curves for sample E242 in Fig.1 and Fig. 2, compared to the experiment.

The *r*-spectra were filtered out in the range 0.5-3.3 Ă and the fit performed in *k*-space. Six single scattering paths (SS) and four multiple scattering (MS) paths were found to be relevant in this range:

- $(Ga\text{-}N)_{//}$, in-plane, I shell path, corresponding to the three Ga-N bonds of the tetrahedron that are nearly in-plane ;
- $(Ga\text{-}N)_{\perp}$, out of plane, I shell path, corresponding to the fourth Ga-N bond of the tatrahedron, lying along c axis;

- $(Ga\text{-}Ga)_{//}$, II shell, in-plane path, corresponding to 6 Ga atoms at a distance equal to *a* cell parameter(in-plane lattice parameter);
- $(Ga\text{-}Ga)_{\perp}$ II shell, out-of-plane path, corresponding to 6 Ga atoms at a distance that is a combination of *a* and *c*, $\{1/3\ a^2 + ¼\ c^2\}^{1/2}$;
- (Ga-N), III shell path, corresponding to one N atom along c direction;
- (Ga-N), IV shell path, corresponding to 6 N nearly in-plane atoms;

The further MS paths consisted of triangular paths Ga-N-N and Ga-N-Ga.
(note: "in-plane" refer to the surface or growth plane)

We performed the fit by letting the lattice parameter *a* and *c* vary but mantaining the hexagonal cell symmetry, i.e. expressing all the interatomic distances of coordination shells, higher than the I one, as a function of a and c. The Ga-N first shell distances were let free to vary independently of a and c since, as it is well known, the Vegard's law is far from being valid for semiconductor alloys, in which the bond-bending mechanism is dominant compared to bond-stretching. The best fit parameters are shown, for the whole set of samples in Table I, where we also report, as a reference, the bulk and pseudomorphic values for GaN.
Starting from the fit results, we calculated the ε_{xx}, $[(a_{sample}\text{-}a_{GaN})/a_{GaN)}]$ and ε_{zz} values, $[(c_{sample}\text{-}c_{GaN})/c_{GaN)}]$, that we sketch in Fig. 3 as ε_{xx} vs ε_{zz} and in fig. 4 as a function of the layers number.
We observe the following findings:

- the Ga-N first shell in-plane and perpendicular-to-plane distances show to be very close to each other, within the fit errors (0.01Å), in agreement with previous studies [2];
- the $(Ga\text{-}Ga)_{//}$ and $(Ga\text{-}Ga)_{\perp}$ II shell distances look to be diffferent, as expected due to the strain effect;
- the $(Ga\text{-}Ga)_{//}$,i.e. *a,* tends to contract as a function of the GaN layers number, approaching the AlN lattice parameter (3.11Å);

In Fig. 3 we compare the GaN elastic behaviour, i.e. $\varepsilon_{zz} = -2\varepsilon_{xx}(C_{13}/C_{33})$, with the experiment. We see that a subelastic trend looks to show. It could be related to the strong piezoeletric effect which tends to compensate the effect of strain, giving lower c values than expected from elasticity [3].

Nevertheless, the ε_x values look to be too high. We must note that the errors on $a_{//}$ are very large (0.06 Å), giving a corresponding large error on ε_x, as shown on Fig. 4. This is mostly due to the lack of data with the beam polarization parallel to the surface that would allow a much more precise determination of $a_{//}$. In addition, the quality of our XAFS spectra is quite poor, the *k*-space range had to be limited to about 10 $Å^{-1}$ due to the presence of numerous Bragg peaks and the signal-to-noise ratio should also be improved. Note that the GaN equivalent thickness is quite low, ranging down to only 6ML for the sample with one QDs layer.

	R1 (Ga-N) (Å)	$R2_{\perp}$ $(Ga\text{-}Ga)_{\perp}$ (Å)	$R2_{//}$: *a* $(Ga\text{-}Ga)_{//}$ (Å)	*c* (Å)	*c/a*
1L (S1582)	1,93	3,18	3,16 *(3,15)*	5,22	1,65
3L (S1580)	1,92	3,16	3,11 *(3,156)*	5,21	1,67
10L (S1581)	1,92	3,16	3,08 *(3,152)*	5,23	1,7
78L (E242)	1,92	3,16	3,08	5,24	1,7
GaN/AlN pseud.	*not available*	3,184	3,11	5,26	1,69
GaN bulk theor.	1,947	3,18	3,18	5,193	1,63

Table I: Best fit results for the measured samples. The statistical errors on the values reported range from 0.01 Å for R1 to about 0.06Å for $R2_{\perp}$, $R2_{//}$ and c. The values reported in parenthesis have been obtained by diffraction measurements

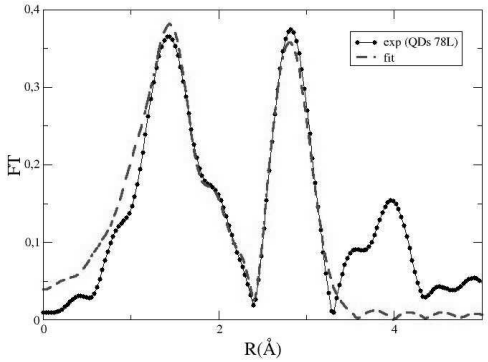

Fig. 2: *R-space best fit results for sample E242*

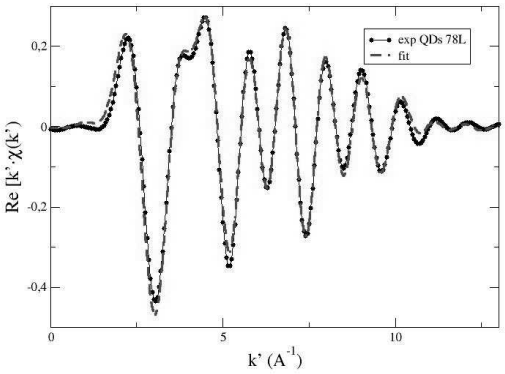

Fig. 1: *k-space best fit results for sample E242*

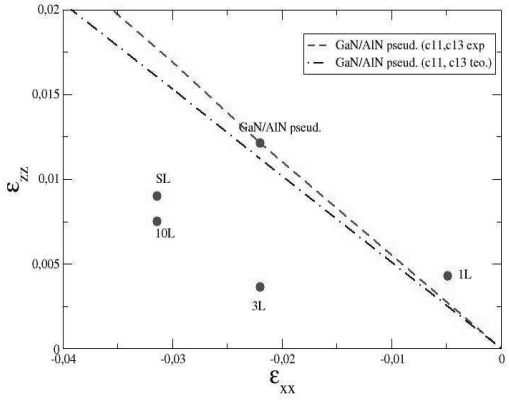

Fig. 3: ε_{zz} *as a function of* ε_{xx} *for the different samples (1L, 3L, 10L, 78L(SL))*

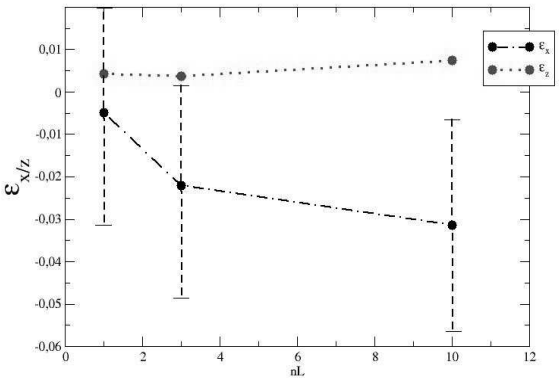

Fig. 4: ε_{zz} *and* ε_{xx} *as a function of the layers number*

In Table I we also show the $a_{//}$ values deduced by X-ray diffraction measurements on the same samples that show to be higher than the EXAFS values. This suggests, as expected, that EXAFS is probing different region of the samples with a uniform weight, that is not the case for diffraction. In particular the wetting layer, that is known to be, in the case of GaN SK growth, a quite consistent part of the total GaN amount (about 2MLs), and it is expected to be pseudomorphic to AlN.

Summarizing, we believe that these preliminary measurements show that EXAFS can provide use valuable information about a system that is being intensively studied and the structural properties of which have not yet been elucidated.

References :

[1] N. Gogneau, D. Jalabert, E. Monroy, T. Shibata, M. Tanaka and B. Daudin, J.Appl. Phys., **94,** 2254 (2003)
[2] F. D'Acapito, f. Boscherini, S. Mobilio, A. Rizzi, R. Lantier, Phys. Rev. B **66**, 205411 (2002)
[3] J. Gleize et *al*., Phys. Rev. B 63,073308 (2001)