	Experiment title: **Study of the incorporation of Rare-earths in GaN/GaInN quantum dots**	**Experiment number**: 30.02.637
Beamline: BM30B	**Date of experiment**: from: 30/10/2003 to: 03/11/2003	**Date of report**: 05/10/2004
Shifts: 12	**Local contact(s)**: Xavier BIQUARD	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Xavier BIQUARD*, CEA-Grenoble - DRFMC/SP2M/NRS

Thomas ANDREEV*, CEA-Grenoble – DRFMC/SP2M/NS

Yuji HORI*, NGK Insulators, Japon (currently in DRFMC/SP2M/NS)

Denis JALABERT*, CEA-Grenoble - DRFMC/SP2M/SiNaPs

Bruno DAUDIN, CEA-Grenoble – DRFMC/SP2M/NS

Report:

Overview

We have recorded room-temperature fluorescence EXAFS and XANES spectra at the Eu, Er and Tm K-edges (6.9 to 9 keV) using the 30-element energy-resolved detector, samples being kept under primary vacuum to avoid air diffusion.

Studied samples were made of 50 layers of doped GaN QDs embedded inside AlN. The QDs were doped with different amount of Eu or Er or Tm, and were grown on an Al2O3 substrate covered by MOCVD AlN as furnished by NGK.

As a lot of Bragg diffraction peaks originating form the substrate were superimposed on absorption spectra, we have systematically used quick-EXAFS scans prior to data acquisition to finely adjust the X-ray incident angle on sample to minimize the number of (annoying) Bragg peaks.

Studied samples

1°) Europium

1. 3 reference samples: metallic Eu sample N0069, bulk GaN doped with Eu (N0042) and Eu2O3 powder.
2. 2 QDs samples: sample S1425 (2.5% of Eu) that was previously studied in IHR, and sample N0066 doped with 0.6% of Eu.

2°) Erbium

1 QDs sample: N0077 doped with 3.2% of Er

3°) Thulium

1. 1 reference sample of metallic Tm N0070
2. 2 QDs samples: sample N0074 (2.3% of Tm) and sample N0073 (3% of Tm)

Results

This proposal was very successful since the good quality of the recorded EXAFS spectra have enabled us to clearly determine the localization of both Eu and of Tm in our samples. Exafs analysis was focused on determining the chemical composition of the second nearest neighbors as is illustrated in figure 1 and table 1 for Eu, and figure 2 and table 2 for Tm. These EXAFS studies (coupled with photoluminescent and cathodoluminescent ones) showed

- that Eu is incorporated substitutionnally inside GaN QDs since only Ga forms the second nearest neighbor shell
- that Tm incorporates substitutionnally at the interface between GaN QDs and AlN, in the AlN part of the interface, thus yielding 1/4th of second nearest neighbors as Ga and 3/4th as Al.

Detailed results concerning Eu were published in "GaN quantum dots doped with Eu", Y. Hori, X. Biquard, E. Monroy, D. Jalabert, F. Enjalbert, Le Si Dang, M. Tanaka, O. Oda, and B. Daudin, APL, vol 84 (2), pp 206-208 (2004)

And detailed results concerning Tm will be submitted shortly (probably to PRB), under the title "Optical and morphological properties of GaN quantum dots doped with Tm", T. Andreev, Y. Hori, X. Biquard, E. Monroy, D. Jalabert, A. Farchi, M. Tanaka, O. Oda, Le Si Dang and B. Daudin.

Second nearest neighbor shell	Eu in GaN QDs	Eu in AlN matrix
Coordination number	12	12
Bond length distortion (%)	-1.7 ± 0.3	- 0.25 ± 1.1
Debye Waller factor (10^{-3} Å^2)	8.3 ± 0.2	4.4 ± 1.2
Energy shift (eV)	-26 ± 2	-10 ± 5
r-factor (quality) of fit (%)	0,14	4

Table 1: best fit parameters for Eu

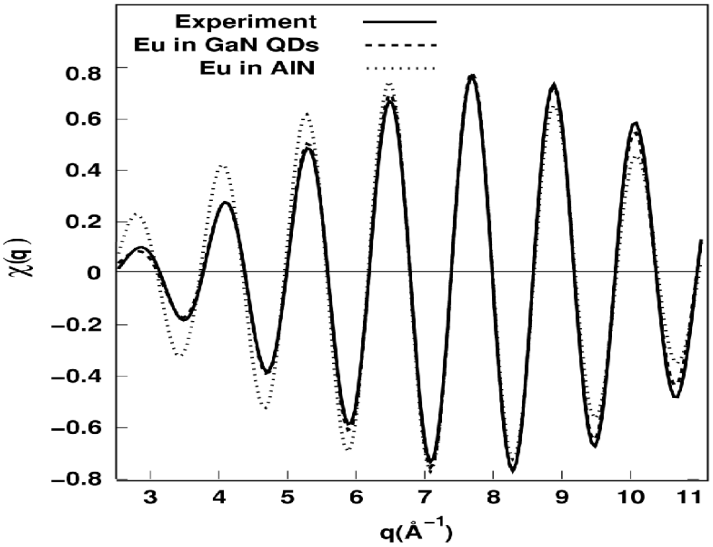

Figure 1: Exafs fits for the second nearest neighbour shell of Eu

Second nearest neighbor shell	Tm in GaN	Tm in AlN	Tm in (GaN,AlN)	
			GaN	AlN
Proportion (%)			25 ± 4	75± 4
Bond distortion (%)	-1.6 ± 0.8	0.0 ± 0.7	-1.7 ± 0.6	+1.8 ± 0.8
DW factor (10^{-3} Å^2)	13± 1	1± 1	5 ± 4	
Energy shift (eV)	-21 ± 4	-6 ± 2	-2 ± 3	
Quality of fit (%)	3,4	3,9	0,2	

Table 2: best fit parameters for Tm

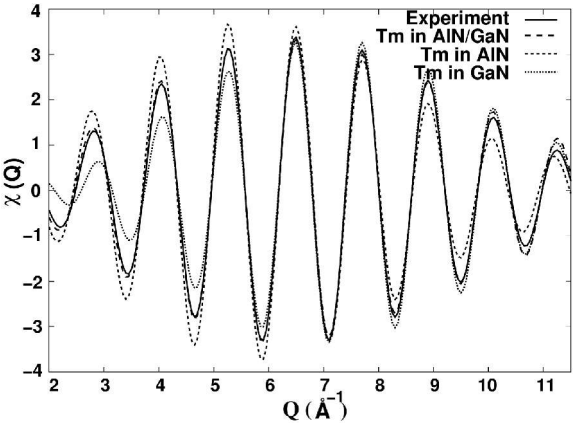

Figure 2: Exafs fits for second neighbour shell of Tm