ESRF	**Experiment title:** Local environment of Gd in GaN: an element with colossal magnetic moment	**Experiment number**: HS3446
Beamline: ID22	**Date of experiment**: from: September 19th to: September 25st 2007	**Date of report**: August 22th 2008
Shifts:	**Local contact(s)**: Gema Martinez-Criado	*Received at ESRF:*

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A set of highly homogeneous GaN:Gd epilayers have been studied by means of XAS and μ-X ray fluorescence at the ID22 microprobe beamline. The purposes of the work were: to analyze the local arrangement of Gd in the GaN host lattice; to clarify the existence of phase mixing; and to obtain the valence of the Gd atom. All these are relevant factors which could contribute to clarify the origin of the unprecedented magnetic moment and high Curie temperatures of this diluted magnetic semiconductor.

In Fig. 1 the XRF data show the L and K shell lines of Gd and Ga, as well as of Ar from the air. The presence of elemental traces such as Si, S, Ca, and Fe is also revealed. By setting regions of interest around the dominant fluorescence lines, the compositional homogeneity was also examined. Uniform patterns with no intensity changes (0.02%) were observed, showing a homogeneous distribution of all significant elements. Whereas impurity aggregation effects are expected and observed in heavily rare earth (RE) doped GaN, our results suggest no tendency to agglomerate at those low Gd levels.

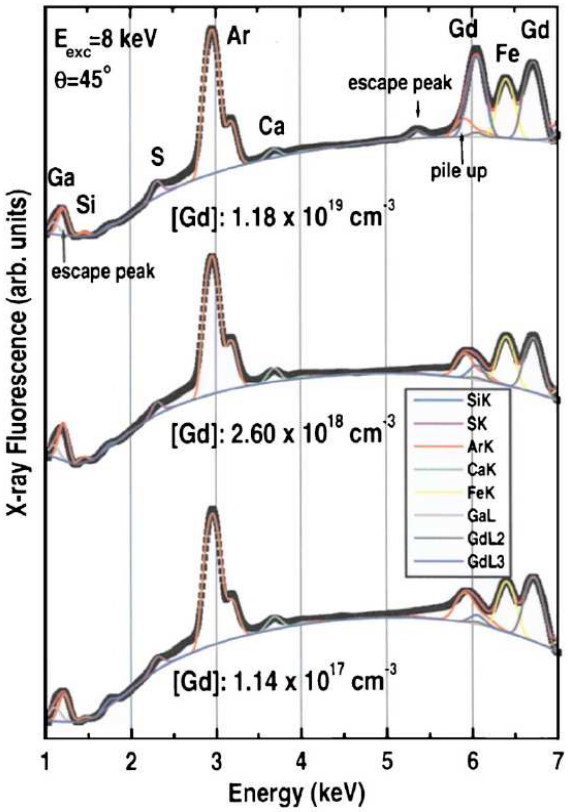

Fig. 1 XRF spectra of GaGdN epilayers.

The XANES data at the Gd L3 edge are plotted in Fig. 2, including for comparison different standards: Gd2O3, Gd foil, and ab initio full multiple scattering simulation by FEFF8 code corresponding to Gd on Ga sites in wurtzite GaN. The spectra exhibit a single prominent resonance mainly from 2p3/2→5d dipole transitions with slight differences on the peak area and halfwidth relative to Gd simulation. From the first derivative of the intensities plotted in the inset of Fig. 2, although Maruyama et al. reported the coexistence of divalent and trivalent RE ions in GaN, here there is no indication of Gd on any other highly lattice symmetry other than the tetrahedral Gd3+ site.

The comparison of the x-ray linear dichroism (XLD) of the XANES at the Gd L3 and Ga K edges provides additional support about the site distributions in the highest Gd doped GaN (0.027%). In Fig. 3 the Gd L3 edge XLD signal is similar to the one observed at the Ga K edge but with smaller amplitudes. The results show a strong anisotropy exhibiting the signature of the hexagonal GaN. There is no remarkable damping effect revealing a strong influence of the Gd impurities in any preferential crystallographic direction.

The weighted radial distribution functions (RDFs) were also obtained performing Fourier transforms of the extended x-ray absorption fine structure (EXAFS) at the Ga K edge (uncorrected for phase shifts). Given the dilute Gd contents, EXAFS collections at the Gd L3 edge were not doable within reasonable acquisition times. We have fitted the neighbor distances Ri and Debye–Waller (DW) factors Si2 of the different atomic shells. The coordination number was fixed to the nominal value for each scattering path, and the amplitude reduction factor S02 was also fixed to be the best-fit value 0.89 for undoped GaN. All the observed RDF contributions provide direct evidence for highly short-range structural order. Within the experimental accuracy, the Ga–N distance is very close to the one in pure GaN (1.94 Å), and that the second neighbor distance virtually equals to the wurtzite lattice parameter (3.19 Å).

In conclusion, we have investigated the chemical and structural properties of MBE-grown GaGdN, revealing Gd ions in a predominantly trivalent state with tetrahedral coordination, occupying Ga sites in the wurtzite structure. Within the sensitivity of our experimental techniques, neither secondary phases nor Ga vacancies were observed.

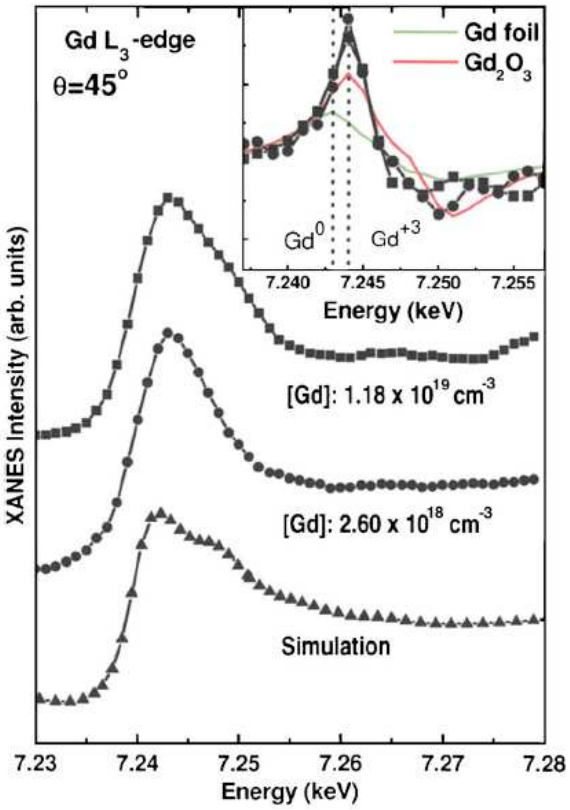

Fig. 2 XANES spectra and the derivatives for the GaGdN layers and various standards.

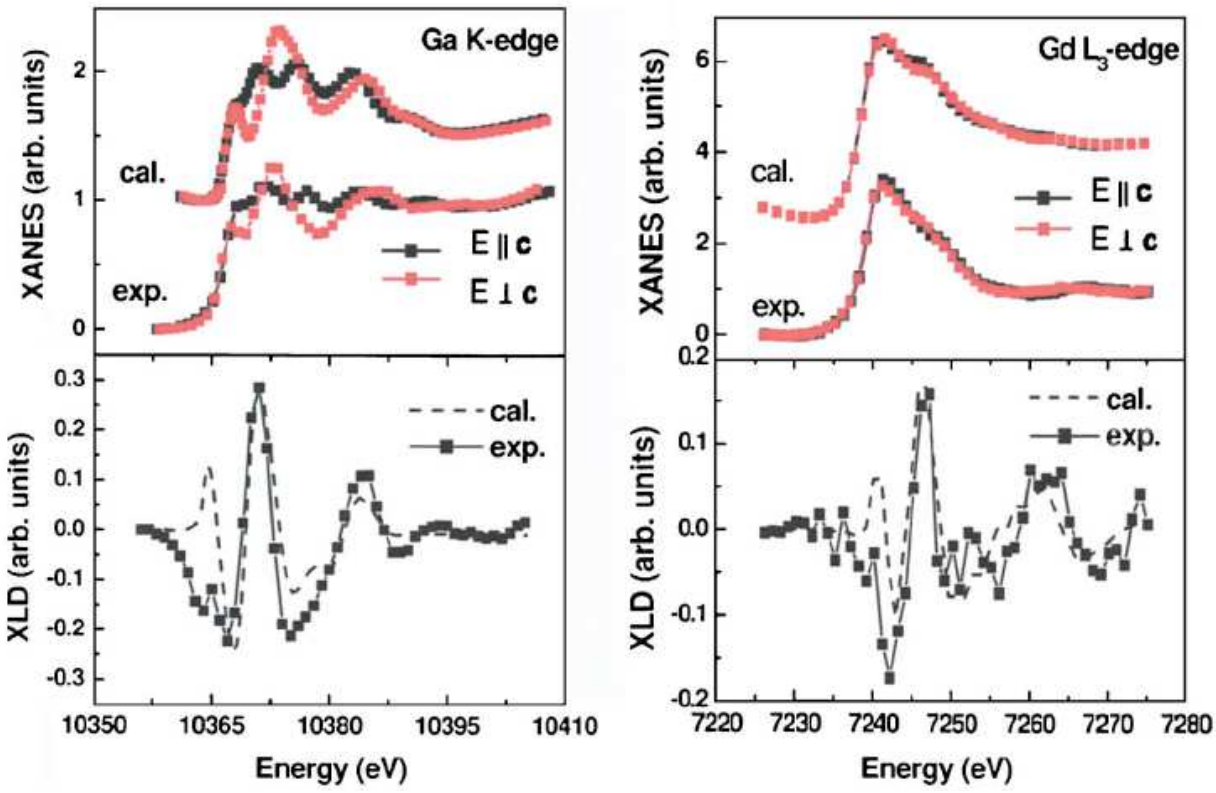

Fig. 3 XANES and XLD signals recorded at the Gd L3 and Ga K edges from GaN with [Gd]=0.027%.The calculated XANES spectra are also plotted with their corresponding XLD.