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The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

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http://193.49.43.2:8080/smis/servlet/UserUtils?start

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Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
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Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** EXAFS study of the local structure of GaMnAs and its changes during annealing	**Experiment number**: HE2470
Beamline: BM29	**Date of experiment**: from: 18.4.2007 to: 22.4.2007	**Date of report**: 28.8.2007
Shifts: 12	**Local contact(s)**: Dr. Sakura PASCARELLI	*Received at ESRF:*

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Report:

Structural properties of diluted ferromagnetic semiconductors such as GaMnAs are of crucial importance for their magnetic performance. In addition to the properties of the averaged GaMnAs lattice (average lattice parameter, structure factors, etc.) that can be studied by x-ray diffraction methods, local structural properties are of importance too, such as local lattice distortion around magnetic ions in substitutional or interstitial positions. In [1,2], these distortions have been studied by x-ray absorption spectroscopy methods (EXAFS and XANES). In our previous work [3] the lattice positions of Mn ions in GaAs and their changes during a post-growth annealing were investigated by the x-ray standing-wave method.

The aim of this work was to study the local structure around the Mn ions in GaMnAs. In contrast to other works in this field [1,2], we have used x-ray absorption spectroscopy in the reflection mode, which allowed us to discriminate between the signal from the sample surface and from the volume of the GaMnAs layer. GaMnAs layers have been grown by MBE on (001) GaAs substrate covered by a thin low-temperature GaAs homoepitactic layer. We have investigated the XANES spectra of a series of samples containing nominally 7% Mn (with the Curie temperature of about 77K) before and after a post-growth annealing at 200°C for 1, 2, and 16 hours. The absorption spectrum was detected by measuring the MnKα fluorescence as a function of the energy of a primary beam for various incidence angles, we have used both a PIN diode and a Ge detector for the fluorescence measurement, placed as close as possible to the sample surface. In order to avoid the elastical-scattering peaks in the spectra, we have limited the measured energy range to approx. 100 eV above the MnK absorption edge.

Figure 1 shows the XANES spectra of a non-annealed and a 16-h-annealed sample before and after HCl etch, measured for various incidence angles around the MnK absorption edge. For both non-etched samples, the shapes of the XANES spectra measured for small and large incidence angle substantially differ. After an HCl dip, the XANES spectra measured at smaller and larger incidence angle become much more similar.

In Fig. 2 we present the XANES spectra of GaMnAs (Mn in substitutional positions) and MnO Manganosite (one of possible Mn oxides). The spectra have been simulated ab-initio using the APW method implemented in the Wien2K program [4], and by two methods (Green-function method and finite-difference method) implemented in the FDMNES program [5]. The FDMNES spectra have been convoluted already by the width of the core state; this is the reason why these spectra are smoother than the spectra from the Wien2K program. From a qualitative comparison of the shape of the measured spectra with the spectra simulated by FDMNES (blue lines in Fig. 2) it follows that the XANES spectrum measured at large incidence angles (i.e., a large penetration depth of the primary radiation) resembles the spectrum calculated for GaMnAs (substitutional Mn). In the case of small incidence angles, the penetration depth of the primary radiation is small and

the XANES signal stems mainly from the sample surface. The shape of the spectra taken at small incidence angles is more similar to the simulated MnO spectrum. In HCl, the surface oxide layer is removed and this is the reason, why the XANES spectra measured after the HCl dip have different shapes.
Further investigations will be focused to a numerical comparison of measured and simulated spectra. We will also investigate theoretically the effect of polarization of the primary x-ray wave on the spectrum. The Wien2K program makes it also possible to relax the positions of the atoms in the neighbourhood of a Mn impurity. Such a shift will affect the simulated XANES spectrum and we hope to determine (at least partially) the local atomic displacements from a detailed comparison of the measured and simulated spectra. Knowing the local lattice distortion, it is also possible to calculate the average structure factor of the lattice and to compare it with structure factors determined from x-ray diffraction.
First results of the analysis of the XANES spectra will be published during next few weeks as a short letter. A more detailed study including also the simulation of the local lattice distortion and the comparison of the simulated and measured structure factors will follow next year.

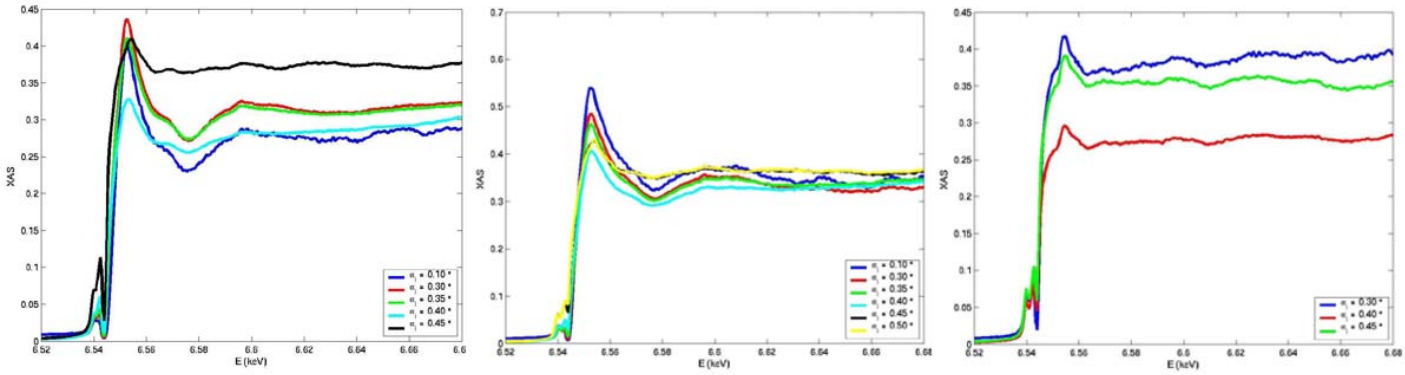

Fig. 1. Measured XANES spectra for various incidence angles, as-grown sample (left), after 16h annealing at 200°C before (middle) and after (right panel) a HCl dip.

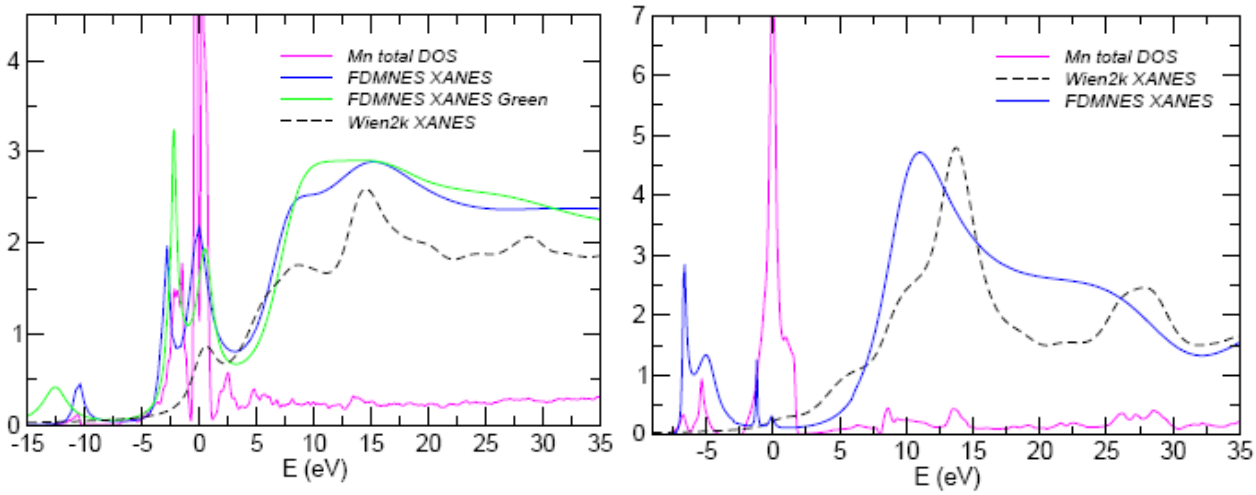

Fig. 2 XANES spectra simulated by the FDMNES and Wien2K programs, and the total density of states (red line) obtained by Wien2K.

[1] A. Titov et al., J. Mag. Mag. Mater. **300**, 144 (2006).
[2] Y. Soo et al., Appl. Phys. Lett. **84**, 481 (2004).
[3] V. Holý et al., Phys. Rev. B **74**, 245205 (2006).
[4] www.wien2k.at
[5] Y. Joly, Phys. Rev. B **63**, 125120 (2001).