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ESRF

Experiment Report Form

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.

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

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

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Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

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All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

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:** X-ray standing-wave investigation of ferromagnetic GaFeN layers	**Experiment number**: SI-1446
Beamline: ID32	**Date of experiment**: from: Sept. 13, 2006 to: Sept. 19, 2006	**Date of report**: February 22, 2007
Shifts: 15	**Local contact(s)**: Dr. Tien-Lin Lee	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Václav Holý, Zdeněk Matěj*, Department of Electronic Structures, Charles University, Ke Karlovu 5, 121 16 Prague, Czech Republic

Rainer T. Lechner*, Inst. of Semiconductor Physics, Kepler University, Altenbergerstr. 69, A-4040 Linz, Austria

Alberta Bonanni, Andrea Navarro-Quezada*, Inst. Of Solid State Physics, Kepler University, Altenbergerstr. 69, A-4040 Linz, Austria

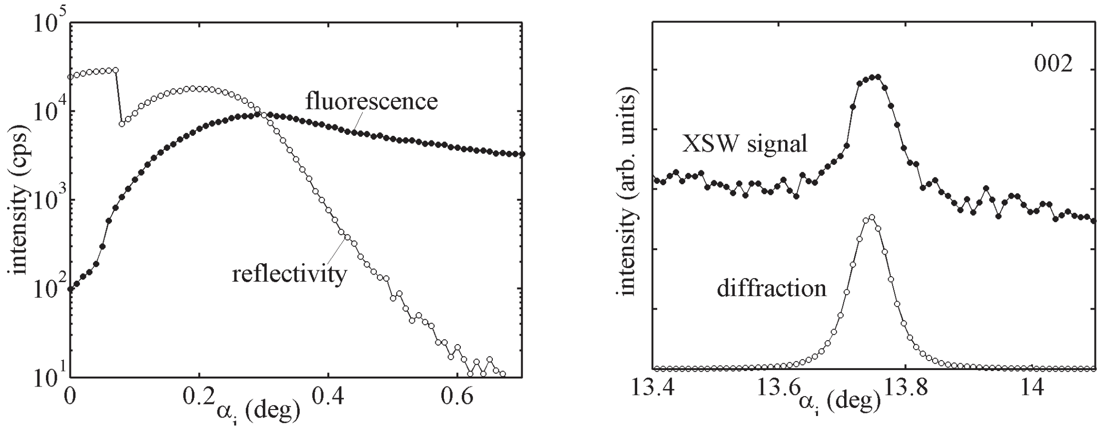
Report:

GaN doped with transition metals is one of the predicted candidates for obtaining Zener-type ferromagnetism with T_c > 300K [1,2]. As a necessary condition, the transition metal ion should be incorporated on isolated (i.e. not clustered) substitutional sites and exhibit a high-spin ground state. So far, the Mn doped GaN has been intensively studied, but it turned out that holes that can mediate the spin ordering in these structures are localized on Mn, therefore Zener-type magnetism is not expected in GaMnN. In this respect, the GaFeN system is much more promising. However, very little is known about the incorporation of Fe in GaN. From secondary ion mass spectroscopy the total amount of iron incorporated into GaN was determined. An electron spin resonance (ESR) study [3] revealed the existence of the charge state Fe^{3+} . From the discrepancy between the two methods we infer that Fe^{2+} is also present at interstitial lattice sites.

The aim of the project was to determine the lattice positions of Fe ions in the wurtzite-type GaN lattice and their dependence on the conditions of epitaxial growth. A series of GaFeN epitaxial layers was grown by metalorganic chemical vapor deposition method (MOCVD) on thick GaN buffer layers deposited on sapphire substrates. In the series, both the thicknesses of the GaFeN layers and the Fe flux in the growth reactor were systematically varied. Magnetic measurements (SQUID magnetometry) revealed a superparamagnetci behavior of these layers with a small ferromagnetic component. For the determination of the lattice positions of the Fe ions, x-ray standing-wave method (XSW) was used, in which the intensity of the FeKα fluorescence radiation was measured as a function of the direction of the primary x-ray wave with the energy of 10.0 keV. Special attention has been paid to a minimization of the fluorescence background originating from Fe-rich parts of the sample holder, slits, collimmators, etc.

For each sample, a series of XSW scans has been measured in various coplanar and grazing-incidence diffractions. Typically, we have used coplanar 002 and 004 diffraction, as well as grazing-incidence diffractions 100 and 110. In the diffraction curves measured simultaneously we did not find only one diffraction maximum – this indicates that the lattice mismatch between the GaFeN layer and the GaN buffer underneath is very small. This fact made it possible to use the standing x-ray wave produced in the GaN buffer for the determination of the Fe positions in the GaFeN layer also in coplanar scattering geometry (see the discussion in [4]). In addition to XSW measurements around various reciprocal lattice points, we have also

measured FeKα fluorescence intensity excited by a primary wave irradiating the sample under very small incidence angle (i.e., during x-ray reflectivity measurements far away from any diffraction maximum). This data make it possible to determine the density profile of Fe atoms in a thin surface layer.
Figure 1 presents some examples of measured curves of sample #596, consiting of a 3 μm thick GaN buffer layer covered by a 50 nm thick GaFeN layer.



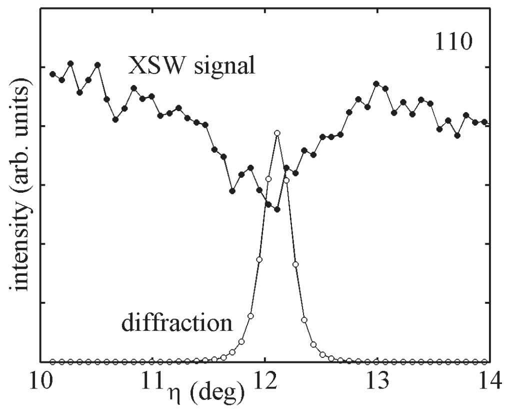


Fig. 1 FeKα fluorescence excited by x-ray reflection (upper left panel), coplanar XSW measurement (upper right) and GID XSW (lower left panel) on GaFeN sample #596. α_i denotes the incidence angle of the primary radiation, η is the azimuthal angle of the primary radiation with respect to the diffracting net planes.

Combining the XSW measurements using various mutualy non-parallel diffraction vectors it is possible to determine all three coordinates of the Fe atoms in the GaN wurtzite unit cell, as well as the coherent fraction, i.e., the relative amount of the Fe atoms in coherent lattice positions [5]. Recently we are working on a theoretical description of the XSW experiment both in coplanar and in a general non-coplanar geometries, based on two-beam dynamical diffraction, as well as on a numerical method for the treatment of experimental data, including a convolution of the simulated XSW curves with an angular resolution function, depending on the optical elements in the primary beam.
The coherent positions and coherent fractions of the Fe atoms determined from the XSW data will be correlated with the magnetic properties of the layers determined previously. A publication of the results is expected in near future.

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[4] V. Holý, Z. Matěj, O. Pacherová, V. Novák, M. Cukr, K. Olejník, and T. Jungwirth, Phys. Rev. B **74**, 245205 (2006).
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