



<b>Experiment title:</b> The x-ray absorption investigation of the GaN: rich-Mn magnetic semiconductors	<b>Experiment number:</b> HE-3928	
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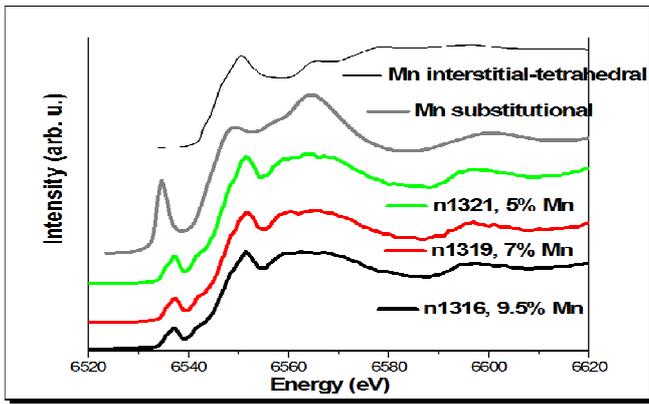
## Report:

The incorporation of Mn in the III-V wide-gap semiconductors matrix, like GaN, results in hole-mediated room temperature ferromagnetism. This effect can be realized by homogeneous diluted magnetic semiconductors (DMSs) with a high concentration of substitutional Mn ions. Nevertheless, the concentration of the Mn ions diluted in III-V semiconductor crystals was for a long time limited to approximately 0.1% by the Mn solubility achieved in equilibrium growth conditions; higher Mn concentrations induce phase separation and surface segregation [1]. Recent progress in MBE growth and in the development of post growth annealing techniques permits to suppress extrinsic effects, pushing  $T_c$  in (Ga,Mn)As up to 173 K [2]. The higher  $T_c$  can be obtained in DMS materials with a higher concentration of substitutional Mn ions [3].

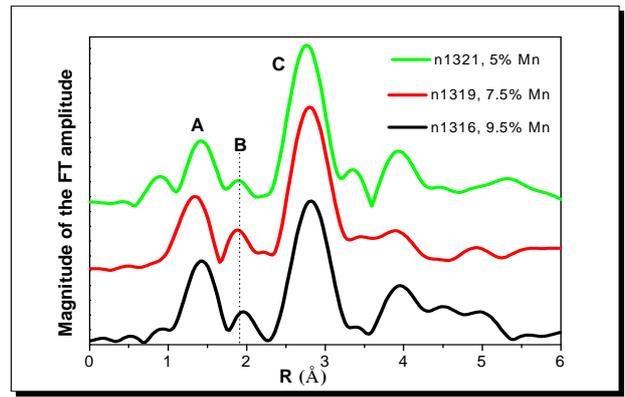
Homogeneous high-Mn-concentration (Ga,Mn)N layers with Mn contents ranging from 1.5 to 9% were successfully grown using molecular beam epitaxy (MBE) method at University of Bremen. Rutherford backscattering investigations performed for samples with the Mn content of up to 7% show that the Mn atoms are placed in the lattice positions (Ga sites). This data and TEM investigations also confirm the high crystalline quality of the samples. Another question arises concerning the nature of the valence state of Mn ions. To determine the valence state of Mn and its lattice positions in the host matrix, x-ray absorption spectroscopy (XAS) methods, such as XANES and EXAFS were used.

An EPI 930 molecular beam epitaxy chamber equipped with a radio-frequency plasma source was used to grow the (Ga,Mn)N layers. During the growth we adjusted the Mn flux so that the growth at the stoichiometric point prevails. A series of five homogeneous samples with Mn contents varying between 1.5 to 9 % was investigated [4].

The XAFS measurements have been performed at the K-edge of Mn:  $E = 6539$  eV in the fluorescence detection mode for two angles of incidence (almost  $90^\circ$  and  $0^\circ$ ). Moreover, the anomalous diffraction was performed. In this measurements the intensity of the GaMnN layer diffraction was measured as a function of the photon energy around the Mn K edge, the measurements have been carried out in diffractions 002 and 103.

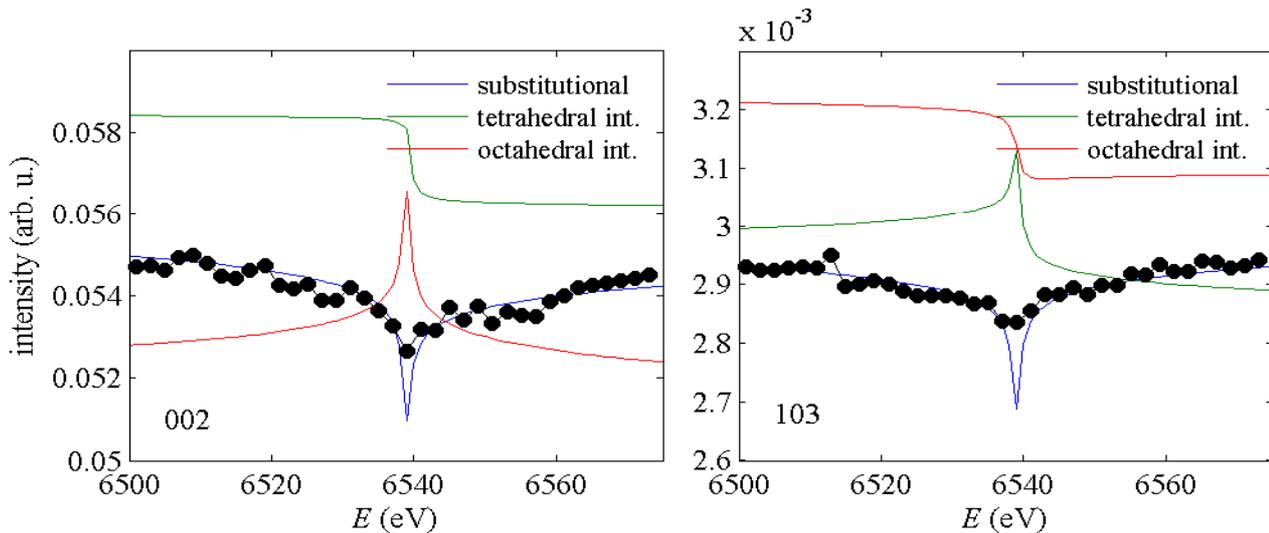


**Fig. 1** The experimental XANES spectra of the Mn K-edge for investigated samples and calculated one for two different models: Mn is in (i) the substitutional (ii) interstitials sites.



**Fig. 2** The module of the Fourier transform of the experimental Mn K edge EXAFS oscillation indicates the existencesome other Mn structure .

The XANES spectra of the investigated samples reveal mainly the features of the spectrum calculated for the model where the Mn atoms occupy the substitutional sites. The pre-edge peak is an indication of the substitutional Mn sites. A single pre-edge peak is characteristic for  $\text{Mn}^{2+}$  ( $d^5$  configuration). Nevertheless there are indication for splitting characteristic for the 3+ charge state. According to the EXAFS data additionally investigation of the presence of the other Mn structure is necessary.



**Fig. 3.** The energy-dependence of the intensities of a  $\text{Ga}_{1-x}\text{Mn}_x\text{N}$  layer,  $x=0.1$ , calculated for various positions of the Mn atoms in the GaN matrix. The dots denote the measured values.

Figure 3 compares the simulated energy dependences of the diffracted intensity for various positions of the Mn atoms in the unit cell, and the measured one. The preliminary results presented here clearly show that the Mn atoms occupy the Ga-substitutional sites and their density is about 10%.

In conclusion, the XAFS and anomalous diffraction confirm the Rutherford backscattering results, namely presence the Mn atoms at the substitutional sites. XANES spectra predict the mixing of two valence states of the Mn impurities, i.e. 2+ and 3+. Due to high sensitivity to the local environment around Mn atoms of the EXAFS method some inclusion of the other Mn phase are observed. This paper reports only preliminary results. Further studies are needed to analyze and understand the data in detail. The electronic structure of the Mn embedded in the GaN matrix help to explain the difference between a theoretically predicted rather high Curie temperature of  $(\text{Ga,Mn})\text{N}$  and its experimental value of only few K. The final results will help to optimise the growth process to the growth of a room-temperature ferromagnetic material.

## References:

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