

Experiment ME-1101: Physical properties and cluster formation in manganese doped GaN with micrometer resolution

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A set of highly homogeneous $\text{Ga}_{1-x}\text{Mn}_x\text{N}$ epilayers have been studied by means of XANES and μ -X ray fluorescence at the ID22 and ID21 microprobe beamlines. The purposes of the work were: to analyze the local arrangement of Mn in the GaN host lattice; to clarify the existence of phase mixing; and to obtain the valence of the Mn atom. All these are relevant factors which could contribute to clarify the origin of ferromagnetism with high Curie temperatures of diluted magnetic GaN [1,2].

From the comparison of the XANES spectra measured around the Ga and Mn K-edge regions [Fig. 1(a)] we observe that the oscillations at the XANES region are practically coincident. Contrary to the GaMnAs, where the Mn atoms frequently appear in interstitial positions at high Mn concentration, in our GaN samples the Mn always substitutes the Ga. The remaining samples show identical oscillations. We have measured the x-ray fluorescence as a function of the angle in order to elucidate

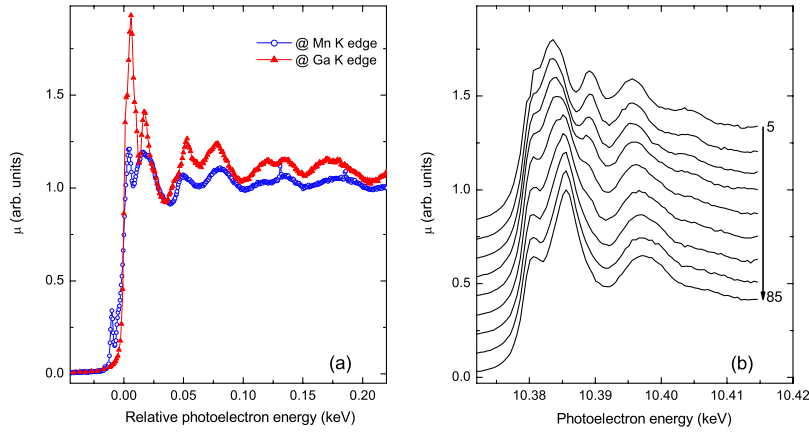


Figure 1: (a) XANES spectra of the 13.7% Mn sample measured at the Ga and Mn K-edges. (b) Angular variation of the XANES spectra of the 13.7% Mn sample measured at the Ga K-edge. The angle step between the different spectra is 10° .

the possible mixing of zincblende and wurtzite phases. Figure 1(b) shows the XANES spectra around the Ga K-edge region, obtained by rotating the sample holder from 5 to 85° . Clearly, there is a shift of the main peak and the peak around 10.39 keV disappears. This is a clear indication of the hexagonal structure, since in cubic symmetry, there is no angular variation.

Nearest neighbors distances [Fig. 2] have been obtained by fitting the Fourier-transformed EXAFS $k\chi$ functions obtained at the Ga and Mn K-edges. The decrease of the Mn-N distance for increasing Mn concentration is consistent with previous X-ray diffraction data showing a decrease in c cell parameter [3].

Figure 3 shows the XANES spectra of the 5.8% sample, measured around the Mn edge at the ID21 beamline. The experimental curve is composed by a pre-edge absorption peak (A_1), consisting of a double peak structure, a shoulder (A_2) and the main peak of absorption (A_3). We have fitted all the

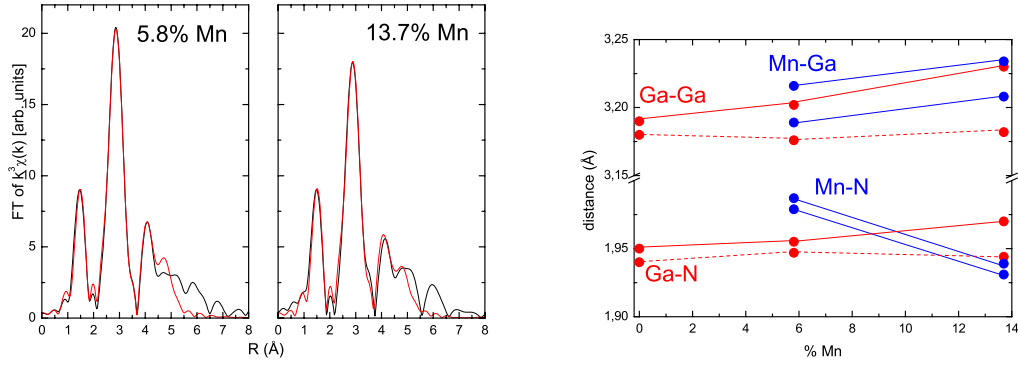


Figure 2: (a) Fourier transform EXAFS compared with the result of fitting (red lines) corresponding to different Mn concentrations. (b) Interatomic distances as deduced from the EXAFS fittings.

experimental data with a multi-Gaussian profile (to account for the disorder). From the derivative we can determine more precisely the position of the edge. An average value of the four samples give $E_{\text{Edge}} \approx 6550.7$ eV. By comparing with the edge position of MnO (Mn^{2+}) and Mn_2O_3 (Mn^{3+}) (the first compound has the edge at 6550.3 eV while the second is located at 6553.8 eV), we obtain a Mn ionization state of 2^+ in all our samples. The pre-edge is due to the transition from the Mn(1s)

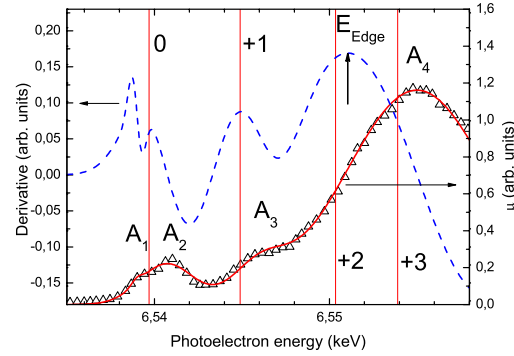


Figure 3: Near-edge region of the absorption spectrum of the 5.8% sample measured at the Mn-K edge. The different structures labeled A_1 (pre-edge), A_2 (shoulder) and A_3 (main peak) are discussed in the text (right scale).

valence band to the t_{2g} anti-bonding states produced by the Mn-N orbital mixing. The shoulder and main peak are due to the corresponding transition to p_x, p_y and p_z states of the conduction band [3].

- [1] H. Hori, S. Sonoda, T. Sasaki, Y. Yamamoto, S. Shimizu, K. Suga, and K. Kindo, *Physica B* **324**, 142 (2002).
- [2] G. Martínez-Criado, A. Somogyi, S. Ramos, J. Campo, R. Tucoulou, M. Salomé, J. Susini, M. Hermann, M. Eickhoff, and M. Stutzmann, *Appl. Phys. Lett.* **86**, 131927 (2005).
- [3] O. Sancho-Juan *et al.*, *Phys. Rev. B*, submitted.