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## Report:

The development of ternary magnetic semiconductors based on III-V compounds is attracting large efforts in view of their potential use in spintronic devices. For example, fabrication of light emitting diodes in which the carriers are spin-polarized has been reported. In such devices, the spin aligner can be made of a Ga(1-x)Mn(x)As magnetic layer embedded in GaAs. An important problem in this materials system is the limited solubility of Mn in III-V semiconductors; in fact, Mn concentration up to 10% can only be achieved by low temperature molecular beam epitaxy (LT-MBE). In order to avoid the formation of MnAs inclusions, the growth temperature for Mn-doped III-V's has to be between 200°C and 300°C, i.e. very low compared to the 500 – 650 °C interval used for standard GaAs-based materials. At such a low temperature the growth of many III-V semiconductors leads to the incorporation of excess anions in the epilayer. Large concentrations of As antisites giving rise to donor states have been observed by cross-sectional scanning tunneling microscopy in $Ga_{1-x}Mn_xAs$. Since ferromagnetic correlation in $Ga_{1-x}Mn_xAs$ is proposed to be mediated by holes, As antisites together with Mn interstitials, which also act as donors, may pin the Fermi level away from the Mn-induced acceptor states thus hindering ferromagnetism.

δ-doping of GaAs with Mn has recently been proposed as one of the alternatives to the growth of bulk $Ga_{1-x}Mn_xAs$ alloys. This method consists in creating a δ-like doping profile in the growth direction by inserting in GaAs a submonolayer thick Mn layer. The basic idea is to achieve locally higher Mn concentrations where high hole densities can be trapped. Electrical activation of Mn and Curie temperature are significantly different with what has been achieved in bulk $Ga_{1-x}Mn_xAs$. The native Mn-induced hole concentration was reportedly insufficient to achieve ferromagnetism, but increasing the hole concentration on the Mn δ-doped layer using a modulation-doped structure containing AlGaAs:Be layers yielded ferromagnetism with an unprecedented Curie temperature of 250 K after annealing, by far the highest reported for this materials system.

In GaMnAs – related materials systems there is a close interplay between the local structure of Mn and the electronic properties. In fact, by using density functional theory simulations, Mahadevan and Zunger have predicted that the formation energy of an interstitial Mn defect decreases as the Fermi level shifts towards the valence band, as can be achieved for example by Be co – doping.

In order to determine the local structure of Mn in δ-doped GaAs layers we have carried out an x – ray absorption spectroscopy (XAS) experiment on the GILDA (BM 08) beamline at the Mn – K edge. Samples were grown on GaAs(001) at the TASC laboratory in Trieste by molecular beam epitaxy with and without Be co–doping; they consisted in a ten – fold repetition of a structure composed of 0.1 to 0.5 monolayers (ML's)

of Mn and a 30 nm GaAs spacer layer; the substrate temperature was 300 °C (samples A1 and A2) and 450 °C (samples B1, B2 and B3). In sample B3 a 0.1 ML of Be was introduced in the GaAs spacer layer in order to lower the Fermi level.

In Fig. 1 we report the magnitude of the Fourier transform of the EXAFS data. All samples, except B3, exhibit the clear spectral signature of the zincblende local structure, suggesting a substitutional site. Sample B3, instead, exhibits very weak second and third shell structures and a significant high – R broadening. In Fig. 2 we report the XANES of sample A1 together with *ab-initio* simulations performed within full multiple scattering theory for substitutional Mn surrounded by Ga atoms and by As atoms.

The EXAFS data have been quantitatively analyzed taking into account the significant single and multiple scattering contributions to the signal. Mn–Mn atomic correlations have not been found within ~ 5 Å radius, ruling out the presence of metallic clusters or local Mn enrichment. In samples deposited at 300 °C, Mn substitutionally occupies the Ga site with a local expansion (≈2%) of the first-neighbor distance with respect to GaAs; the second neighbors remain at a distance very close to that of host lattice, indicating that the structural perturbation induced by Mn is very localized. *Ab – initio* simulation of the X-ray absorption near edge structure spectra (Fig. 2) confirmed that Mn enters the Ga, rather than the As, site. Samples grown at 450 °C exhibit a reduction of the first shell coordination number, suggesting the initial phases of MnAs precipitation. In the case of Be co-doping the downward shift of the Fermi level leads to the appearance of Mn in tetrahedral interstitial sites (which cause the high – R broadening in Fig. 1), of which we provide a previously unavailable local structural description.

These results have been published in F. D'Acapito, G. Smolentsev, F. Boscherini, M. Piccin, G. Bais, S. Rubini, F. Martelli, and A. Franciosi, Phys. Rev. B **73**, 035314 (2006).

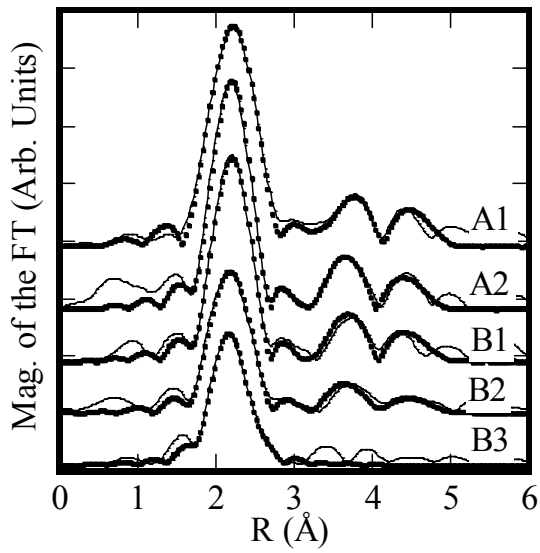


Fig. 1

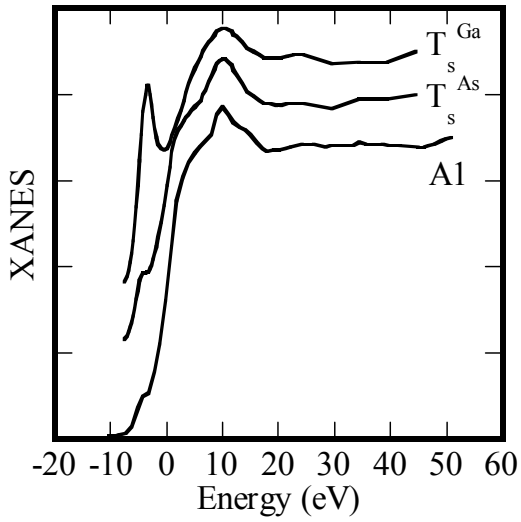


Fig. 2