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# Ga INTERSTITIAL SITE OCCUPATION BY Mn ATOMS IN GaAs: EXAFS AND XANES EVIDENCE

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A significant amount of scientific activity is devoted to studies of Mn containing semiconductors. In particular, $Ga_{1-x}Mn_xAs$ is considered as a promising material for microelectronic applications utilizing the electron spin. The location of the Mn atoms in the layers, here grown by means of MBE, is correlated with all relevant physical properties of the final material, and is therefore the subject of many studies. To avoid MnAs segregation, the MBE growth of (Ga,Mn)As must be performed at temperatures which are much lower than those normally applied (550 - 650ºC) for GaAs, *i.e.* at 180 - 300ºC, depending on Mn content [1]. $Mn^{2+}$ ions with spin 5/2, substituting for Ga in this material, are ferromagnetically coupled due to exchange interactions with valence band holes, giving rise to the ferromagnetic behavior of $Ga_{1-x}Mn_xAs$. Substitutional Mn ions ($Mn_{Ga}$) act as acceptors, generating holes that mediate the ferromagnetic exchange [2]. However, a low (MBE) growth temperature leads to a high density of point defects [3]. The most important of them are known as As anti-sites ($As_{Ga}$) [4] and Mn interstitials ($Mn_i$) [5] which are double donors significantly compensating a fraction of free holes. A powerful tool for the determination of the Mn location in layer is X-ray Absorption Spectroscopy (XAS), as it probes the local atomic order and the electronic structure [6, 7]. Here we present a study of the Extended X-ray Absorption Fine Structure (EXAFS) and the X-ray Absorption Near Edge Structure (XANES) of MBE grown $Ga_{1-x}Mn_xAs$ layers.

XAS measurements were performed at liquid nitrogen temperature, at the A1 experimental station in HASYLAB (Hamburg, Germany) using a double crystal Si (111) monochromator. The Mn K-edge spectra were registered using a seven-element fluorescence Si detector. The Mn L-edges spectra were measured at MAX-lab (Lund, Sweden) at beamline D1011 applying total electron yield detection.

To analyse the EXAFS and XANES spectra different Mn positions within the GaAs matrix were considered: (i) substitutional $Mn_{Ga}$, (ii) interstitial (As) – with As atoms as the first neighbours, (iii) interstitial (Ga) – with Ga atoms as the first neighbours. Due to the fact that electron scattering on Ga and As atoms is very similar, the differences between different Mn position in the EXAFS spectra were not noticed within the first coordination sphere but only considering also the further neighbourhood. The analysis of up to the third sphere with only the substitutional Mn position resulted in the fit of the model to the experimental spectrum presented in Fig. 1.

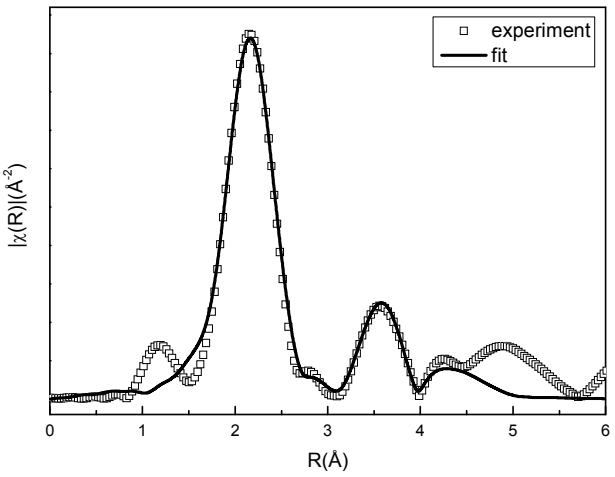


Figure 1. Modulus of the Fourier-transformed $k\chi(k)$ functions (squares) and fit (solid line) for the substitutional Mn position.

Making this assumption, it has been impossible to fit the experimental spectra around 5 Å. Considering the possibility of Mn location in the interstitial (Ga) – with Ga atoms as the nearest neighbours, allowed to simulate experimental data successfully (Fig. 2). The number of Mn atoms in this position was comparable with the one in the substitutional position.

This finding was additionally verified by ab initio calculations of the influence of the Mn atom location on the shape of the XANES spectra [8]. The calculations were performed using the FEFF 8.4 code. The theoretical predictions were compared with the experimental K and L edge XANES of Mn. The results of the performed simulation and the comparison with the XANES Mn spectra for the K as well as for the L edges confirmed that a substantial part of Mn atoms should be located in the Ga interstitial position.

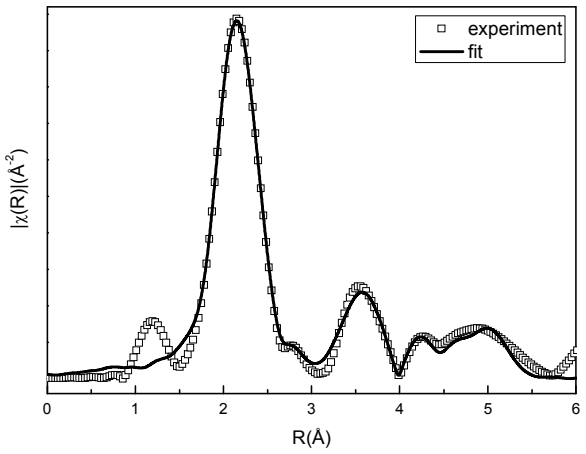


Figure 2. Modulus of the Fourier-transformed $k\chi(k)$ functions (squares) and fit (solid line) for the substitutional and the interstitial (Ga) Mn position.

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