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Structural evolution of (Ga,Mn)As thin film during medium temperature post growth annealing manifested by XAS

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An extensive research is currently being conducted to develop a diluted magnetic semiconductor (DMS) with room temperature ferromagnetism and proper transport properties, qualities desired for future spintronics devices. (Ga,Mn)As is the most studied DMS material and with the optimized MBE growth and post growth annealing procedures the Curie temperature, T_C, as high as about 200 K has been achived, see, e.g., [1] where the results of different heat-treatment conditions are presented. A comprehensive understanding of the microstructure evolution on transformation processes (including formation and migration of point defects) which occur in (Ga,Mn)As during growth and post growth annealing could potentially lead to a further progress in reaching higher T_C. The goal of this work is to add to this understanding by checking the effectiveness of X-ray absorption spectroscopy as a probe of structural evolution of (Ga,Mn)As after medium temperature post growth annealing (up to 450 °C).

The (Ga,Mn)As layer was grown in a SVTA MBE system [2] on GaAs (100) substrate with thin AlAs buffer layer. An amorphous As capping layer was deposited on (Ga,Mn)As at the end. After removing from the MBE setup, the film was cleaved into three pieces: one piece was left intact and the other two were annealed at temperatures 350 °C and 450 °C. After conventional initial analysis, the (Ga,Mn)As layer was separated from the GaAs substrate on all samples by chemical etching, a so-called "lift-off" procedure [3], in order to avoid disturbance of X-ray absorption measurements by Bragg scattering of the bulk GaAs substrate at defined values of energy of incident beam.

The content of Mn in the $Ga_{1-x}Mn_xAs$ layer was estimated to be ~1 at.% by Energy-dispersive X-ray spectroscopy (EDX) using Auriga 40 FIB-SEM workstation. High resolution diffraction studies were performed using a Philips X'Pert-MRD diffractometer equipped with a parabolic X-ray mirror, a four-bounce Ga 220 monochromator at the incident beam, and a three-bounce Ge analyzer at the diffracted beam. The qualitative analysis of ω/2θ scans obtained for the symmetric (004) reflection for the annealed samples allows to manifest the structural reorganization in (Ga,Mn)As film. It is assumed that initially Mn atoms form 'N-mers' which is followed by transition to Mn-rich areas in GaAs matrix, like inclusions.

In order to determine the electronic and atomic structure around Mn atoms the XAFS spectra at the K-edge of Mn were gathered at the BL22 CLÆSS beamline at ALBA synchrotron light facility [4]. Figure 1 presents normalized XANES spectra around Mn K edge and an inset shows modulus of Fourier transforms, FT(R), of the EXAFS function for the samples.

The quantitative analysis of XANES and EXAFS of the "as-grown" sample indicates that Mn atoms most likely substitute Ga atoms in the GaAs matrix. For the annealed samples, a dramatic decrease of the amplitude of FT(R) function can be satisfactory explained by changing in either of these highly correlated parameters: an increase in Debye-Waller factor (accounting for structural and thermal disorder) will result to the same effect as a decrease in number of the atoms in corresponding coordination shell, e.g. by forming As vacancy/ies around Mn atom in the 1st shell. To test the latter hypothesis a possibility to form a specific type of point defect including, for instance, V_{As}, Mn_{Ga}, and their combinations, was estimated by calculating their formation energies using Quantum Espresso DFT code. The structures with the defects with the lowest formation energies were used by FEFF8 multiple-scattering code to calculate theoretical XANES spectra. It was found that reasonable combination of several theoretical spectra provide good qualitative agreement with the experimental ones. In addition, as the hypothesis directly implies the existence of vacancies in (Ga,Mn)As, positron annihilation measurements are planned to estimate type and amount of vacancies in the samples allowing to correlate them with the observed by XAFS effects.

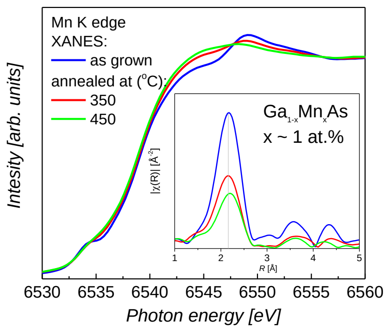

Figure 1. Normalized Mn K-edge XANES spectra of the (Ga,Mn)As layers. The inset shows Fourier transforms of the k^1-weighted Mn K-edge EXAFS χ function.

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