ESRF	**Experiment title:** Hydrogen in ferromagnetic semiconductors: Influence on the structural and electronic properties	**Experiment number**: HS 2726
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ESRF

Report:

We investigated the influence of hydrogenation on the local lattice structure of the ferromagnetic semiconductor $Ga_{1-x}Mn_xAs$. Hydrogen was incorporated by a remote DC plasma with the samples held at 170°C during the hydrogenation. Successful hydrogenation was verified by the disappearance of ferromagnetic resonance and spin wave excitations. As control samples, $Ga_{1-x}Mn_xAs$ samples annealed at the same temperature without a plasma were used. Mn K-edge (6.539 keV) X-ray absorption spectra were collected at room temperature in fluorescence mode by means of a 13-element Ge hyper-pure solid-state detector. The EXAFS data analysis was performed following conventional procedures. Using the FEFF code we simulated, starting from a model atomic cluster, the amplitudes and phases shifts for all single and multiple scattering paths up to the third coordination shell. Subsequenly, we fitted the bond lengths R_i and Debye-Waller factors σ^2_i of the different atomic shells.

Fig. 1 shows a comparison of the Fourier transforms of the Mn K-edge EXAFS $k^*\chi(k)$ functions of an as-grown, a hydrogenated, and an annealed piece of sample B413 (x = 0.04). The spectra look very similar, except for a reduced magnitude of the nearest As-neighbor peak around 2.2 Å (distance not corrected for the phase shift) for the hydrogenated sample. This observation is confirmed by the results of corresponding measurements performed on a second sample B421 (x = 0.04, not shown). This amplitude reduction is accounted for by the significant increase of the nearest As-neighbor Debye-Waller factor σ^2_{As} of the hydrogenated sample shown in Fig. 2(d). The fits also indicate an increase of the second and third shell Debye-Waller factors σ^2_{Ga} and σ^2_{As2} for the hydrogenated samples [Fig. 2(e) and 2(f)]. The physical meaning of the Debye-Waller factors rise is an increase of local structural disorder after hydrogenation.

Theoretical models of the Mn-H complex suggest a bond-centered position of the H atom in between two neighboring Mn and As atoms with an increase of the corresponding Mn-As distance by about 0.7 Å with respect to non-hydrogenated $Ga_{1-x}Mn_xAs$ [A. Amore Bonapasta, F. Filippine, and P. Giannozzi, Phys. Rev. B **72**, 121202(R) (2005); J. P. Goss and P. R. Briddon, Phys. Rev. B **72**, 115211 (2005)]. From these results, since the complete disappearence of ferromagnetic properties upon hydrogenation suggests that a relevant fraction of Mn-As bonds should be streched, we would have expected an additional shoulder on the higher distance side of the nearest As-neighbor peak for the hydrogenated sample in Fig. 1 in case of formation of the predicted defect. However, such a shoulder can not be resolved for any of the two samples investigated. In contrast, we only observe a slight increase of the nearest As-neighbor bond length R_{As} [Fig. 2(a)]. Therefore, our measurements do not corroborate the theoretical predictions.

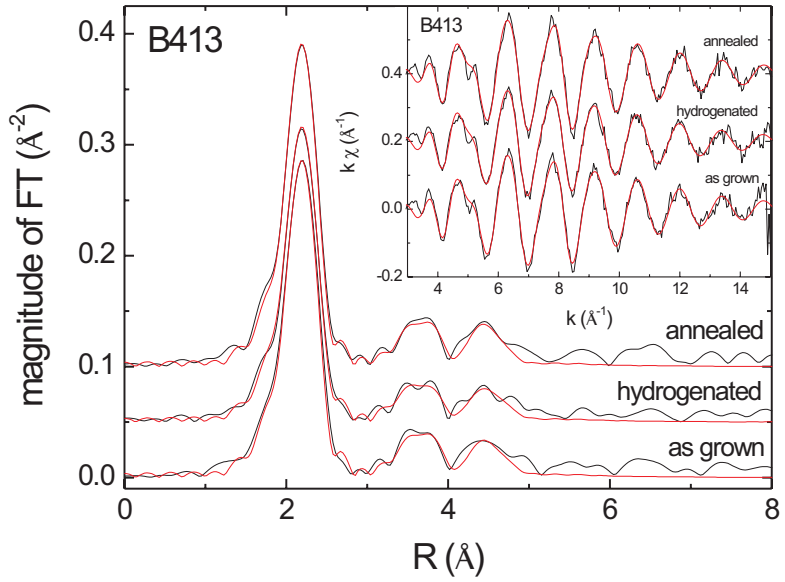

Fig. 1: Comparison of the Fourier transforms of the Mn K-edge EXAFS χ functions of an as-grown, a hydrogenated, and an annealed sample. The red curves are fits to the measured data. The inset shows the k-weighted Mn K-edge EXAFS χ functions. For clarity, the curves have been shifted vertically.

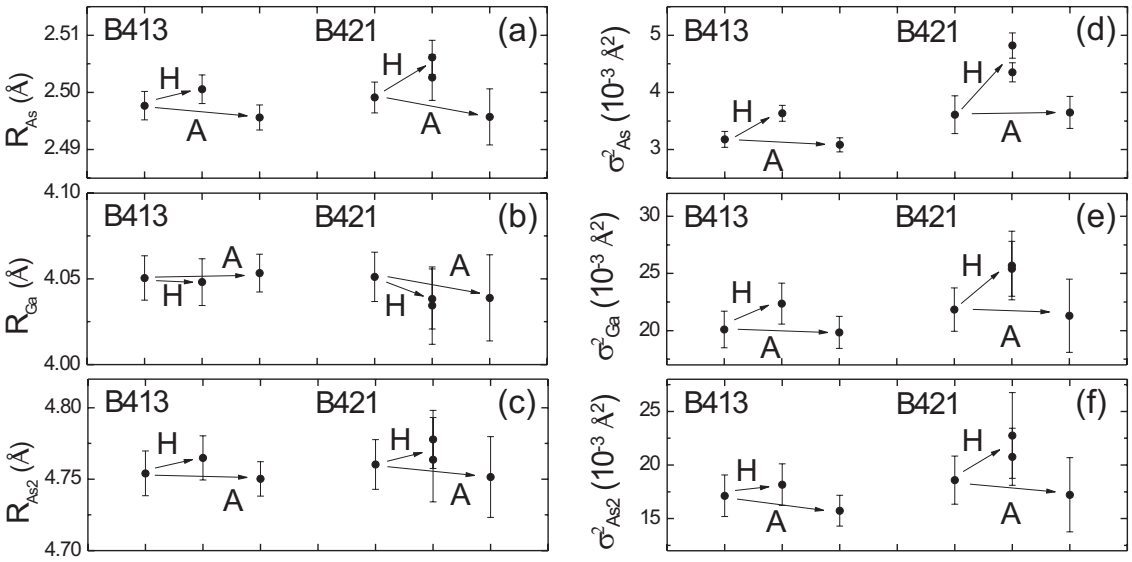

Fig. 2: (a) Nearest As-neighbor bond length R_{As}, (b) nearest Ga-neighbor bond length R_{Ga}, and (c) second nearest As-neighbor bond length R_{As2}, as well as (d) nearest As-neighbor Debye-Waller factor σ^2_{As}, (e) nearest Ga-neighbor Debye-Waller factor σ^2_{Ga}, and (f) second nearest As-neighbor Debye-Waller factor σ^2_{As2} as a function of sample treatment (H = hydrogenation; A = annealing) determined from the fits to the spectra obtained on sample B413 in Fig. 1 and on sample B421.