ESRF	**Experiment title:** Study of the interstitial site of Mn in (Ga,Mn)As films by grazing incidence x-ray absorption spectroscopy	**Experiment number:** HS3345
Beamline: BM08	**Date of experiment:** *from:* 2007-12-12 *to:* 2007-12-17	**Date of report:** 2008-03-05
Shifts: 12	**Local contact(s):** Francesco D'Acapito	*Received at ESRF:*

Names and affiliations of applicants (⋆ indicates experimentalists):
Mauro Rovezzi⋆, CNR-INFM-OGG GILDA CRG c/o ESRF, Grenoble
Francesco D'Acapito⋆, CNR-INFM-OGG GILDA CRG c/o ESRF, Grenoble
Jacek K. Furdyna, Department of Physics University of Notre Dame, USA
Xinyu Liu, Department of Physics University of Notre Dame, USA

Report

Grazing Incidence X-ray Absorption Fine Structure (GIXAFS) experiment has been conducted at the Italian CRG beamline "GILDA" (BM08) on a series of $Ga_{0.94}Mn_{0.06}As$ diluted magnetic semiconductors produced at the department of Physics of Notre Dame university (USA). The experiment has been conducted in fluorescence mode at Mn K-edge (6539 eV) in the GIXAFS dedicated station (ReflEXAFS). During the allocated 12 shifts, Extended X-ray Absorption Fine Structure (EXAFS) specta have been collected on a series of six samples as summarized in Tab. 1. Samples presents good reflectiviy ($\approx 75\%$) as shown in Fig. 1(a). In order to collect informations from the surface and the bulk, fluorescence spectra have been collected at two geometrical configurations: total reflection (TR), $\theta_{TR} = 0.80\theta_c$ and high incidence (HI), $\theta_{HI} = 1.20\theta_c$, where θ_* are incident angles and θ_c is the critical angle. During the energy scan, the choosen work angle has been kept fixed and the reflectivity signal monitored. To increase the signal-to-noise ratio many spectra have been collected on each sample and averaged. Unfortunately spectra presents distortions (due to standing-waves) and contaminated by Bragg Peaks, expecially for those collected at high incidence angle.

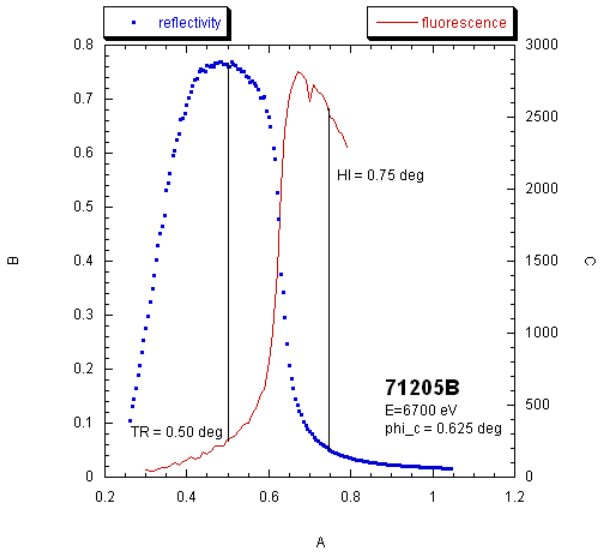
Sample		spectra		$Oxide$ (%) ±5	R_O (Å) ±0.02	σ^2_O (Å^2) ±0.003	R_{As} (Å) ±0.01	σ^2_{As} (Å^2) ±0.001
71205B *GaAs capping layer 2.2 nm*	AS	TR	5	34	2.07	0.016	2.50	0.002
		HI	1	0	-	-	2.50	0.003
	AN	TR	6	58	2.14	0.014	2.58	0.014
		HI	4	40	2.05	0.019	2.48	0.002
71205C *GaAs capping layer 6.0 nm*	AS	TR	6	0	-	-	2.49	0.002
		HI	1	0	-	-	2.50	0.004
	AN	TR	6	0	-	-	2.49	0.004
		HI	0	-	-	-	-	-
71205D *GaAs capping layer 0 nm*	AS	TR	1	51	2.07	0.014	2.51	0.004
		HI	0	-	-	-	-	-
	AN	TR	1	47	2.11	0.007	2.54	0.027
		HI	1	36	2.05	0.014	2.51	0.002

Table 1: Series of $Ga_{0.94}Mn_{0.06}As$ thin layers (133 nm) deposited by low-temperature molecular beam epitaxy (LT-MBE) on GaAs (001) substrates. Each samples, as deposited (AS), has been cleaved into two pieces; one of them has been annealed (AN) at 285 °C for 70 min in N_2. On the left are reported the number/conditions of collected spectra during the experiment and on the right part results from the quantitative analysis.

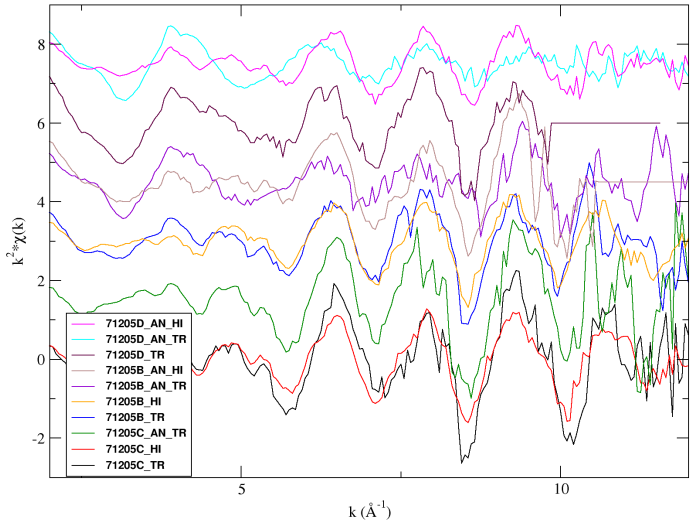
EXAFS oscillations have been extracted using the VIPER software and are showed in Fig. 1(b). Data analysis has been conducted with the IFEFFIT package - containing ATHENA and ARTEMIS softwares - in the Fourier transformed R-space obtained filtering the k^2-weighted $\chi(k)$ signal using Hanning window in the k-range [3.0–9.0] Å^{-1} with dk=1. Two theoretical models have been used in the quantitative analysis generating scattering

paths with the FEFF software: substitutional Mn in zinc-blende GaAs; Manganese oxide. Experimental data have been fitted up to third coordination shell in the R-range [1.0–5.0] Å and main results (relative to the first coordination shell) are reported in Tab. 1 with two representative fits showed in Fig. 2.

The main results found from this preliminary analysis are that GIXAFS is a well suited surface technique and is highly sensitive to oxide presence on the surface. It is clearly visible that only the 6nm capping layer prevent MnO formation in both as deposided and annealed sample; on the other hand, this is not true for 2.2nm and 0nm capping layers were oxide phase dominate the signal. Another important result is the Mn-As distance expansion for total reflection data in annealed samples that present oxide at surface. In fact, Mn-As moves from the usual 2.50 Å typical of Mn dilution in GaAs to 2.56 Å that is the typical distance in case of MnAs precipitation. In addition the high expansion of Mn-O distance could be interpreted as a Mn-Mn dimers contribution. Unfortunately the low quality of the collected spectra and the presence of additional phases have not permitted to distinguish the presence of Mn in interstitial sites and their mechanism of surface migration with the annealing process. For these reasons more experimental investigations are needed on this topic.



(a) Reflectivity (%) and fluorescence (counts/s) signals for sample 71205B as a function of the incident angle (deg) at a given energy (6700 eV).



(b) EXAFS oscillations extracted from collected and averaged spectra as indicated in Tab. 1

Figure 1: Experimental data

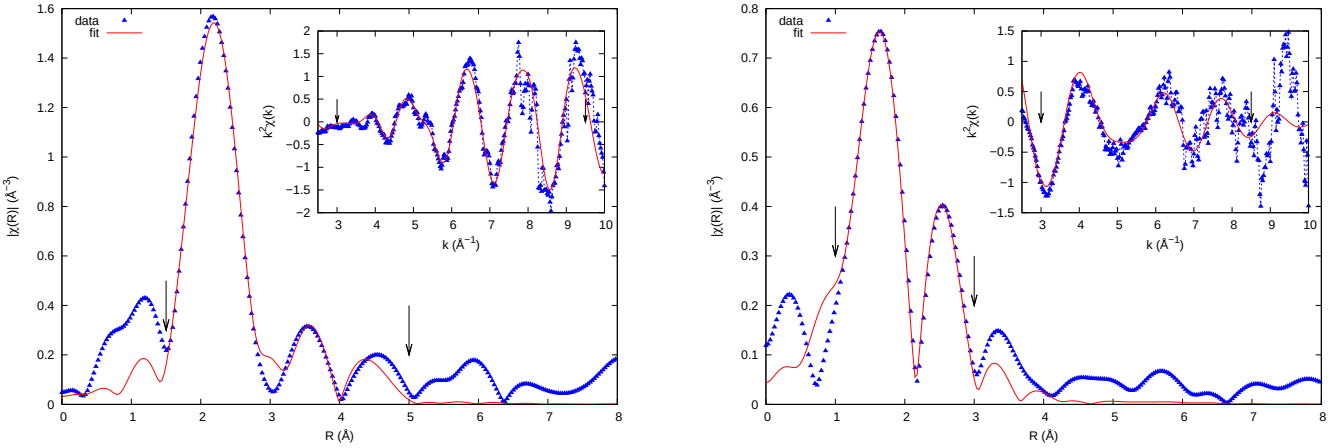


Figure 2: Total reflection data and fits: k^2-weighted EXAFS (inset) and relative Fourier tranforms for samples 71205C_AN (left) and 71205B_AN (right). Arrows indicate fit ranges.