Atomic Structure of Mn on InAs (100)

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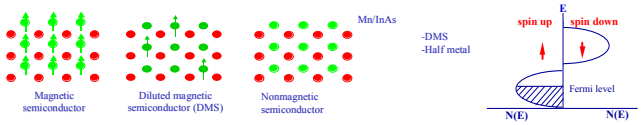
Introduction

A new category of semiconductors, called diluted magnetic semiconductors (DMS), are alloys between a nonmagnetic semiconductor and a magnetic element (manganese in most cases).
An important property of these materials is that the carrier density can be controlled over a wide range between n- and p- types. This opens up the possibility to control magnetic properties simply by changing the carrier density. This behaviour is generally called "carrier-induced ferromagnetism" because hole carriers introduced into the system mediate the ferromagnetic coupling between Mn ions.
So, in such systems, both, the charge and the spin of the electron can potentially be used to create new types of semiconductor devices.



Experimental data

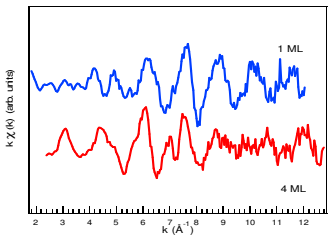


Fig1: EXAFS spectra after background substraction of Mn/InAs for 1 and 4 m.l. of mangannese recorded at the Mn K-edge.

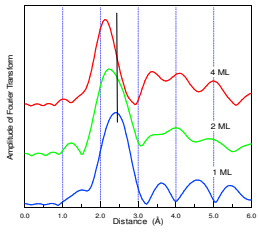


Fig2 : Fourier transforms of the EXAFS spectra of Mn/InAs for three different Mn amounts.

The overall shapes of the EXAFS oscilllations on fig.1 are different in these two films. The vertical bar indicates the first nearest neighbour positions in the sample 1ML of Mn. This distance is obviously longer than for 4 ML of Mn.

results

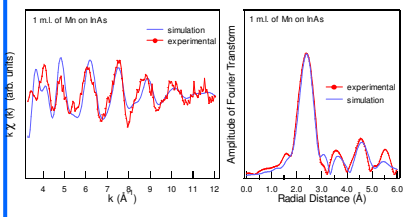


Fig 5 : EXAFS oscillations of one monolayer of Mn on InAs. Comparison with experimental with calculated results

Fig 6 : Fourier Transform of one monolayer of Mn on InAs. Comparison with experimental with calculated results

Comparison between experimental EXAFS spectra (fig 5) of 1 m.l. of Mn deposit on InAs (100) and theoretical spectra generated by In-site-substitution structure ($In_{1-x}Mn_xAs$ compounds in zinc-blende structure) with parameters given in table II.

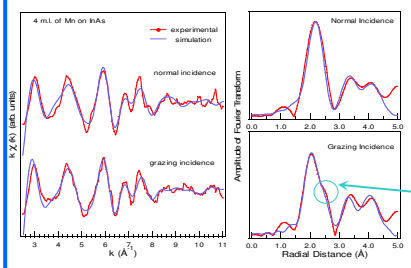


Fig 7: EXAFS oscillations of 4 monolayers of Mn on InAs. Comparison with experimental with calculated results

Fig 8 : Fourier Transform of 4 monolayers of Mn on InAs. Comparison with experimental with calculated results

Comparison between experimental EXAFS spectra (fig 7) of 4 m.l. of Mn deposit on InAs (100) and theoretical spectra generated by MnAs structure (hexagonal packed structure NiAs type), with parameters given in table II, in normal and grazing incidence.

For this sample the best fit value was obtained with the MnAs structure averaged in all directions (we have a polycrystalline MnAs film).

Nevertheless the fact that we see a difference between normal and grazing incidence spectra (Fig 8) shows that there is a preferential crystal orientation. To take account of this we added in grazing incidence a small contribution of monocrystalline contribution (Fig 4)

Experimental

In the surface EXAFS experiments in fluorescence detection, we have studied the growth mode of Mn on InAs(100)c(8x2). We present the results on three sample 1,2, and 4 monolayers of Mn deposited at 530 K. At this temperature there is a strong diffusion of Mn atoms and formation of $In_{1-x}Mn_xAs$ compounds.

Taking advantage of linear polarization of synchrotron radiation, we have measured the EXAFS signal in normal and grazing incidence to enhance or cancel the weight of contribution of each bond to the total signal. We can measure a possible anisotropy in the local order around Mn atoms.

Simulations

Two structures are possible:
$In_{1-x}Mn_xAs$ compounds in which In atoms are substituted by Mn atoms and thus the zinc-blende structure of InAs is conserved.
MnAs compounds with hexagonal packed structure (NiAs type).

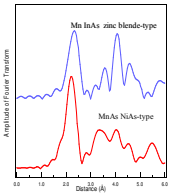


Fig 3 : Fourier Transform of two types of structures

Model calculations based on the MnAs structure and InAs structure with parameters given in table I. The EXAFS spectra were generated by FEFF6 programs.
A direct comparrison of the Fourier Transform (Fig 3) show the different structure, moreover the position of the first pics coresponding of the first nearest neighbour (FNN) are not at the same position.

In the EXAFS formula the coordination number is given by:

$3\sum_{j=1}^{N_i}\cos^2\alpha_j$ where α_i is the angle between the polarization of the X-Ray and bond between the central atom (Mn) and FNN (As and Mn).

The weight of each bond in EXAFS oscillations can be enhanced or canceled by changing this angle.

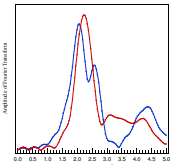
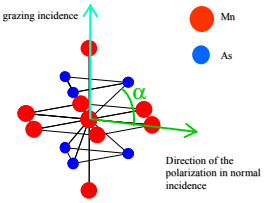


Fig 4 : Fourier Transform of EXAFS spectra in normal (red) and in grazing incidence (blue)



In MnAs structure, the theoretical EXAFS oscillations for the two directions are different. We plotted (Fig4) the Fourier Transform of EXAFS spectra simulated in normal and grazing incident.

Tables

Central atom	Neighboring atom	N	R (Å)
Mn in MnAs	As	6	2.57
	Mn	2	2.85
	Mn	6	3.71
	As	6	4.51
	Mn	12	4.68
	As	6	4.78
In in InAs	As	4	2.61
	In	12	4.27
	As	12	5.00

Table I : Structural parameters for MnAs and InAs (N is the coordination number and R is the interatomic distance).

Sample		First neighbor		Second neighbor		Ratio of coordination
		r_{Mn-As} (Å)	σ_{Mn-As} (Å)	r_{Mn-As} (Å)	σ_{Mn-As} (Å)	N_{As}/N_{Mn}
1 m.l.		2.64	0.1	...	...	4 / 0
4 m.l.	Normal	2.61	0.117	2.865	0.154	6 / 1.8
	Grazing	2.60	0.097	2.864	0.129	6.1 / 1.8

Table II : Best fit values of parameters for 1 monolayer of Mn on InAs and 4 m.l. on InAs in normal and grazing incidence

conclusion

Quantitative analysis of the spectra indicates that for low Mn deposition (1 ML) manganese atoms replace In atoms in the InAs monocrystal, whereas for larger amounts (4ML) the MnAs compound is preferentially formed.

MnAs compound is mainly polycrystalline but a small monocrystalline contribution subsists in grazing incidence measurements, showing that this sample is not perfectly isotropic .