XAFS studies of the local structure of Mn doped dilute magnetic semiconductors

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In recent years a rapid development of spintronics is observed. The goal is to create conceptually new devices which will utilize spin of electron. To achieve this goal it is necessary to fabricate effective injectors of polarized spin and to learn how to manipulate the spin and detect it.

The great expectation is put in so called diluted magnetic semiconductors (DMS). The desired ferromagnetic semiconductor should have the Curie ($T_c$) temperature above the room temperature and have the capability to create material with $n$- and $p$- type of conductivity in the same crystal. One of the example of such a material is extensively studied GaAs with Mn added as the magnetic material. The highest ferromagnetic phase transition temperature ($T_c$) reported so far in GaMnAs is close to 170 K, for GaMnAs containing about 8% of Mn. $T_c$ is proportional to the Mn content and to the concentration of valence band holes. High $T_c$ can be achieved in the material from which compensating defects are removed during the post-growth annealing procedures. The composition of GaMnAs is limited to about 10% Mn due to the Mn segregation into MnAs precipitates observed above this limit.

These precipitations were considered as a drawback up to now. However, since MnAs is a metallic ferromagnet with $T_c$ of about 40°C, the GaAs:MnAs granular system constitutes an interesting material with small ferromagnetic nanoparticles immersed in the semiconductor host lattice. Such a composite material could be considered as a good semiconductor (applicable for integrated circuits) filled with small magnets providing built-in magnetic field at room temperature. This field would affect semiconductor band structure, in particular, leading to differentiation of semiconductor spin states, which is essential for a spintronic material.

We have studied the GaAs:MnAs samples with different Mn contents prepared under different conditions. In order to determine the local atomic structure around Mn atoms we analyzed the EXAFS spectra at the K-edges of Mn for GaAs:MnAs as well as for the reference homogeneous GaMnAs alloys. After growth the samples were subsequently annealed at the temperatures 500 and 600°C, respectively (the details of the growth of the similar structures are described in [1]).

The position of Mn atoms in the zinc-blende lattice of Ga$_{1-x}$Mn$_x$As has a crucial role in determining the magnetic properties of the material. Substitutional Mn atoms occupying gallium sites (Mn$_{Ga}$) act as acceptors and contribute to the ferromagnetic ordering. On the other hand, manganese atoms in the interstitial positions (Mn$_{I}$) are double donors which decreases the hole concentration and destroys the ferromagnetism [2]. In [3] it was shown (on basis of the investigation of Mn-doped GaAs structures by STM) that two types of Mn-related dopants in the sample were observed: 1) those involving only Mn substitutional(s), including both isolated and pairs of substitutionals and 2) complexes composed of substitutional and interstitial Mn.

For examination of the local structure around Mn atoms inside GaAs host under different growth conditions the EXAFS technique was applied. Measurements were done at the A1 experimental station in HASYLAB using the double crystal Si (111) monochromator at the liquid nitrogen temperature. The experiments were performed at the K-edge of Mn (6539 eV) applying seven-element Si fluorescence detector.

As example, in Figure 1 modulus of the Fourier transforms (FT(R)) of the EXAFS spectra for the reference and the investigated samples (as grown and annealed at 600°C) are presented. One can clearly see the differences in the radial distribution function around Mn central atom (particularly in the region of 3-5 Å). In Figures 2, 3 comparison between FT(R) for the investigated samples and theoretical models (Mn$_{Ga}$ – substitution model where atoms of Mn replace Ga atoms in GaAs host; MnAs(cub) – model corresponding to cubic structure of MnAs; MnAs(hex) - model corresponding to hexagonal structure of MnAs) is shown.
From comparison of the experimental data for the investigated samples with theoretically obtained curves we conclude that thermal annealing gives rise to temperature-dependent variations in the local structure around Mn. For the as grown film, the EXAFS analysis indicates that Mn atoms most likely substitute Ga atoms in GaAs matrix. The bond lengths $R_{\text{Mn-As}} = 2.485 \pm 0.004$, $R_{\text{Mn-Ga}} = 4.01 \pm 0.01$, $R_{\text{Mn-As}} = 4.71 \pm 0.01$ and number of atoms 4As, 12Ga and 12As in the 1, 2 and 3 coordination shells around Mn central atom are close to the parameters for bulk Ga$_{0.99}$Mn$_{0.01}$As sample. The substitution model (MnGa) describes the local structure around Mn central atom in “as grown” sample quite well with the $R_{\text{factor}} \sim 0.04$. Looking for the better model, at present, the approach combining the substitutional and the interstitial models is considered.

After annealing of the sample (600°C) the average bond lengths ($R_{\text{Mn-As}} = 2.570 \pm 0.004$, $R_{\text{Mn-Ga}} = 2.852 \pm 0.023$, $R_{\text{Mn-Mn}} = 3.721 \pm 0.015$, $R_{\text{Mn-As}} = 4.541 \pm 0.017$) become similar to that in the hexagonal MnAs. The numbers of atoms in corresponding coordination shells (1-4) are changed (in comparison with “as-grown” sample) and are equal to 6As, 2Mn, 6Mn and 6As ($R_{\text{factor}} \sim 0.01$). This confirmed that after annealing at 600°C the MnAs hexagonal inclusions were formed.

References


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