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$s, p - d$ EXCHANGE CONSTANTS OF CdFeSe SEMIMAGNETIC SEMICONDUCTOR *

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We report determination of $s, p-d$ exchange constants for hexagonal CdFeSe combining exciton splitting and magnetization measurements performed on the same samples.

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Fe-based Semimagnetic Semiconductors (SMSC) have attracted considerable interest during recent years [1]. In particular $s, p - d$ exchange interaction was studied in cubic ZnFeSe [2] and hexagonal CdFeSe [3, 4]. In the latter case exchange integrals were estimated based on exciton splitting and low field susceptibility [4]. In this paper we report results of more reliable way of determining exchange parameters using exciton splitting and magnetization measurements.

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Experiment

The $Cd_{1-x}Fe_xSe$ crystals were grown by the modified Bridgman method. We studied the samples of Fe mole fraction $x \leq 0.13$. We measured reflectivity and transmission in the free exciton energy range at temperature $T = 1.9$ K. Magnetic field ($B \leq 5$ T) was oriented relatively to the hexagonal c-axis of the crystal.

Magnetization measurements were performed in the same temperature and field configuration using the very same samples.

Results and discussion

In the absence of magnetic field two exciton lines (A and B) are observed, as expected for hexagonal crystals [5]. Representative exciton splittings for different magnetic field orientation are shown in Fig. 1a, b. These splittings are in general

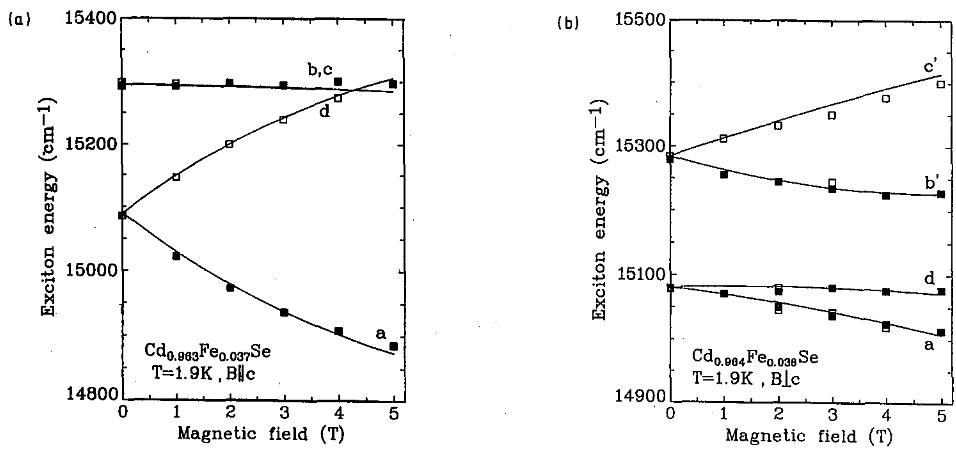

Fig. 1. Energies of the exciton lines (a, b$-\sigma^+$; c, d$-\sigma^-$) in $Cd_{1-x}Fe_xSe$ at $T = 1.9$ K for: (a) B parallel to the crystal hexagonal axis and $x = 0.037$; (b) B perpendicular to the crystal hexagonal axis and $x = 0.036$; the lines show results of theoretical calculations with $N_0\alpha = 0.23$ eV and $N_0\beta = v - 1.6$ eV.

similar to those found for CdMnSe [5], however exciton level field dependence is characteristic for Van Vleck-type paramagnetism of Fe^{++} ions. Strong exciton anisotropy resulting from hexagonal symmetry of the crystal is observed.

Having in mind similar exciton behaviour in Mn- and Fe-based SMSC, we describe $s, p-d$ exchange interaction in CdFeSe assuming the exchange Hamiltonian in a similar form as for Mn–SMSC

$$H = -Js_{e,h} < s_z > xN_0. \tag{1}$$

In (1) J is the exchange operator resulting in matrix elements $\alpha =< s|J|s >$ and $\beta =< x|J|x >$ for conduction and valence bands, respectively; $s_{e,h}$ is the

z-component of band electron (hole) spin; $< s_z >$ is the mean value of Fe ion spin, and N_0 denotes the number of unit cells per unit volume.

The fact, that magnetization of Fe^{++} ions results from both spin and orbital momenta [4] is taken into account by introducing the coefficient κ into the relation between the mean spin $< s_z >$ and macroscopic magnetization:

$$< s_z > = \kappa \frac{m}{x} \frac{1}{\mu_B} M_m, \tag{2}$$

where $m = (1-x)m_{\mathrm{Cd}} + x m_{\mathrm{Fe}} + m_{\mathrm{Se}}$ is the mass of CdFeSe molecule and M_m is the magnetization (per unit mass). In the case of CdFeSe $\kappa = 0.444$ [4] (while for spin-only case $\kappa = 1/2$).

The exchange parameters $N_0\alpha$ and $N_0\beta$ can be determined by combining exciton splitting data with magnetization data in the configuration $B \parallel c$. In this case the splitting of lines a and d (Fig. 1a) reads [4]:

$$\Delta E = E_{\mathrm{d}} - E_{\mathrm{a}} = (N_0\alpha - N_0\beta)\kappa M_m \frac{m}{\mu_B}. \tag{3}$$

In Fig. 2 we demonstrate that, in fact, the exciton splitting in CdFeSe is a linear function of macroscopic magnetization, similarly as it was encountered in ZnFeSe [2] and Mn-based SMSC. The presented experimental data for all the

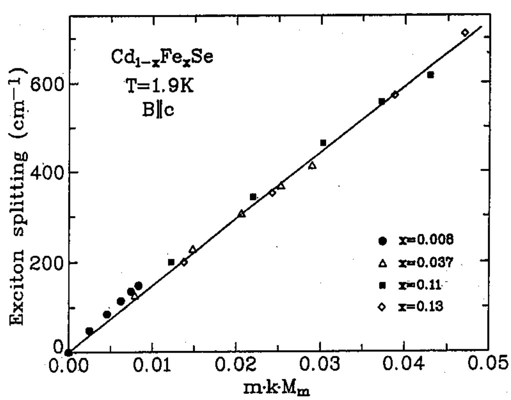

Fig. 2. Exciton splitting for $B \parallel c$ versus magnetization for $Cd_{1-x}Fe_xSe$. The straight line is plotted for $N_0\alpha - N_0\beta = 1.85$ eV.

samples were fitted by a single straight line with a slope ($N_0\alpha - N_0\beta$) = 1.85 eV. This value is slightly smaller than previous estimates based on susceptibility measurements (2.1 eV [4]). Using $N_0\alpha = 0.225$ eV (resulting from Raman scattering experiment) we obtain $N_0\beta = -1.62$ eV, which is comparable to the ZnFeSe value (–1.75 eV [2, 4]), and is substantially higher than CdMnSe value (–1.26 eV [5]).

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