SUPEREXCHANGE INTERACTION IN $A^{II}B^{VI}$–BASED SEMIMAGNETIC SEMICONDUCTORS

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In this report Mn^{2+}, Fe^{2+} and Co^{2+} ions in the ground state in the presence of crystalline field T_d symmetry are considered. Superexchange interaction is performed via S, Se, Te ions. Theoretical calculations of the superexchange interaction integral J_{NN} have been carried out within the framework of Racah technique. Experimental values of J_{NN} for $Cd_{1-x}Fe_xTe$ were obtained from the measurement of Faraday rotation temperature dependence.
Key words: semiconductors, superexchange, Faraday effect.

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A number of properties of semimagnetic semiconductors (SMS) of $A^{II}_{1-X}M_XB^{IV}$ type (where M — Mn, Fe, Co) is determinated by the exchange interaction of localized magnetic moments with band carrier spin [1]. In these structures in addition to the mentioned interaction other mechanisms of magnetic moment exchange are possible. In particular, there is direct exchange associated with the direct overlap of the wave functions of magnetic ions. This mechanism is essential for high concentrations of x of the magnetic component M. At low concentrations of x the exchange between magnetic ions is realized through indirect exchange mechanisms. For the wide band SMS that are studied in this paper the superexchange through the intermediate nonmagnetic is substantional [2]. As concentrations of x are increased magnetic ions may form certain complexes (clusters). Energy characteristics of such clusters are determined by the exchange integral J_{NN}. The quantity of J_{NN} is studied by means of experimental investigations on Raman scattering, magnetization in magnetic field, nonelastic neutron scattering, specific heat [3]. Theoretical analysis of the exchange interaction of J_{NN} is based upon the phenomenological Heisenberg Hamiltonian

$$H = -\sum_{i,j} J_{ij}\mathbf{S}_i\mathbf{S}_j. \tag{1}$$

In (1) due to significant decrease of the interaction with distance ($J_{ij} \sim \exp(-R_{ij})$) the summation is carried over the first neighbours only. In (1) for the case of s-electrons only exchange part is taken into account. The generalization of Heinzeberg model is important for the many electron system with orbital states taken into account [4].

In this paper the effects of superexchange interaction for the structures with M being Mn, Fe, Co and nonmagnetic ion being S, Se, Te are considered. Besides, the role of orbital effects in exchange interaction is investigated and the limits of applicability of Heisenberg Hamiltonian are found. Theoretical analysis of known experimental results [3] is carried out. We also found J_{NN} from the study of Faraday effect for $Cd_{1-x}Fe_xTe$.

In semiconductor solid solutions $A^{II}_{1-x}M_xB^{VI}$ the magnetic component M replaces the cation A and is subject to a crystalline field of T_d symmetry that is formed mostly by the first neigbour anions. Let us single out the M–B–M system in the lattice and consider superexchange interaction of magnetic ions M via nonmagnetic ion B. Many electron states of isolated atoms are described in L–S coupling approximation. For an atom containing N electrons in $3d$-shell a quantum state is described by the set of quantum numbers SLM_SM_L. Crystalline field is taken into account through an appropriate unitary transformation

$$\Psi_{CF} = \hat{U}\Psi_A. \tag{2}$$

The expression for $\hat{U}$ is given in [5], Ψ_{CF} is the basis of wave functions in the presence of crystalline field and Ψ_A is the basis of atomic wave functions. We neglect direct interaction between magnetic ion electrons and treat the exchange part of Coulomb interaction between ions M and B as a perturbation to the system of magnetic ions in ground state. In terms of antisymmetrization operator [6] it corresponds to taking into account permutations $P_{ia}P_{jb}$ (i,j and α,β correspond to the magnetic and nonmagnetic centers respectively). The expression for superexchange operator is obtained in [7]. The calculation was carried out according to the Heitler–London model with the implementation of the Racah technique. This approach does not require the band spectrum charge carriers unlike that in [4].

Theoretical calculation consist in the computation of two-center exchange and overlap integrals with the use of one-electron Slater wave functions [8]. For the simplification of numerical calculations the radial parts of the wave functions were approximated by the set of Gauss functions

$$R_n(r) = \sum_i c_i\phi_i(r), \quad \phi_i(r) = r^{n-1}e^{-\alpha_i r^2}. \tag{3}$$

Material	Mn		Fe		Co	
	Theory	Experiment	Theory	Experiment	Theory	Experiment
CdMTe	6.6	6.2	26.7	24.3±2		
CdMSe	9.6	7.6, 8.1	24.8	19.0	44.2	37.0
CdMS	7.2	9.7, 11.0	18.3		26.0	
ZnMSe	15.0	12.3	25.5	22.3	56.3	49.5
ZnMS	19.4	16.1	31.2	>22.0	53.5	47.5

Table. Superexchange interaction integral $J_{NN}(K)$.

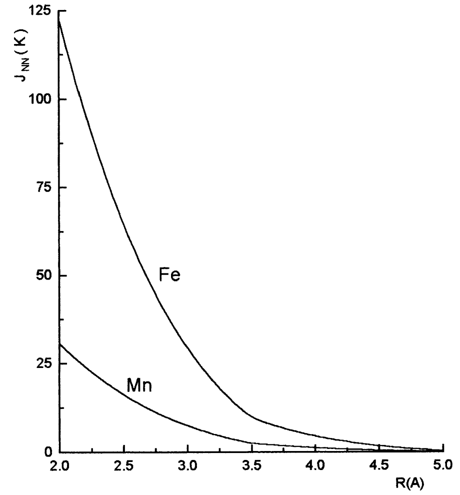

Fig. 1. Integral J_{NN} as a function of distance between magnetic ions.

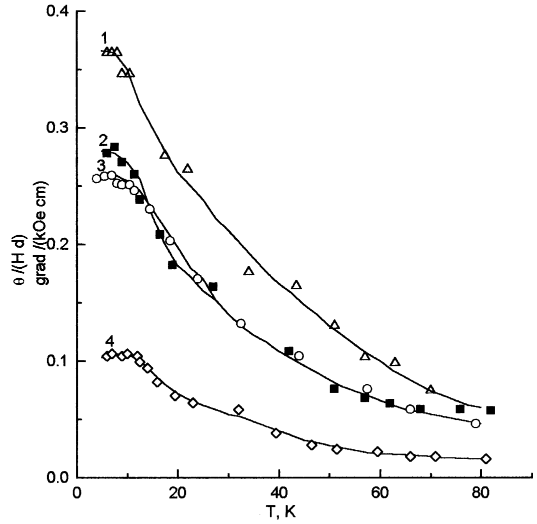

Fig. 3. Temperature dependence of the Verdet constant for $Cd_{0.97}Fe_{0.03}Te$ crystal of different concentrations: 1) $x = 0.01, E$=1.512 eV; 2) $x = 0.03, E$=1.494 eV; 3) $x = 0.05, E$=1.494 eV; 4) $x = 0.03, E$=1.512 eV.

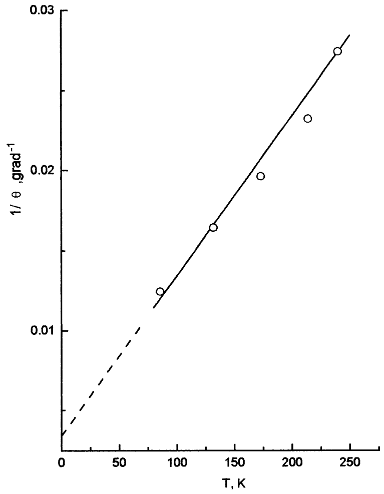

Fig. 2. Temperature dependence of the inverse Faraday rotation angle for $Cd_{0.97}Fe_{0.03}Te$; H = 15 kOe, d = 0.1 cm, $E/E_0 = 0.9$.

Parametrs c_i, α_i were found according to the least square method [8].

Numerical calculation show that the terms which correspond to the nonzero orbital moment are significantly smaller than the corresponding spin terms. It means that Heisenberg Hamiltonian is a sufficiently good approximation for magnetic ion interaction. The results of calculations for J_{NN} are shown in the table. One can see that J_{NN} is subsantially dependent on the type of magnetic ions and increases in the sequence Mn, Fe, Co which is in good agreement with experimental data [3]. Qualitatively these results can be explaned by the fact that screening parameter α being essentially the only parameter of the problem is chosen according to the well-known Slater rule for an isolated atom. The absolute value of J_{NN} is rather sensitive to the choice of α. In order to reach the quantitative agreement with experimental values of J_{NN} [3] α was altered within $\pm 20\%$ of the value of α for an isolated atom. However, it should be noted that the ratio $J^{\rm Fe}_{NN}/J^{\rm Mn}_{NN}$ is only slightly sensitive to the change of α.

The results shown in the table are valid for a fixed value of distance between the magnetic ions. The value of superexchange integral for Fe-Te-Fe and Mn-Te-Mn as a function distance between magnetic ions is shown in fig. 1. For the distance $\sim a/2$ the ratio of superexchange interaction integrals reads $J^{\rm Fe}_{NN}/J^{\rm Mn}_{NN} \sim 3$.

In order to determine J_{NN} for $Cd_{1-x}Fe_xTe$ we used the method of extrapolation of temperature dependence of inverse Faraday rotation angle Θ_F. Example of temperature dependence of inverse Faraday rotation angle for $Cd_{1-x}Fe_xTe$ with $x = 0.03$ (fig. 2) shows that in the interval $70 < T < 250$ K the Courie–Weiss relationship is valid. By means of extrapolation of the linear interval we obtained the value of $\Theta_0 x = -(35 \pm 3)$ K. Using a well-known relationship

$$\Theta_0 = -8S(S+1)J_{NN} \tag{4}$$

we found $J_{NN} = (24 \pm 2)$ K. This value is consistent with the theoretical calculations.

The nature of temperature dependence of the Faraday rotation for low temperatures 4.4<T<70 K (fig. 3) is more complex. The peculiarities of helium at liquid temperatures are due to Van–Fleck paramagnetism [9]. It can be noted that critical value of concentration of x at which interionic exchange interaction becomes substantial for $Cd_{1-x}Fe_xTe$ according to [10] is ~ 0.3 whereas our investigation for $Cd_{1-x}Fe_xTe$ gives $x \sim 0.03$. In other words superexchange interaction for $Cd_{1-x}Fe_xTe$ is essentially greater at a given concentration than it is for $Cd_{1-x}Fe_xTe$ which is consistent with the calculation data (fig. 1).

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НАДОБМІННА ВЗАЄМОДІЯ В НАПІВМАГНЕТНИХ НАПІВПРОВІДНИКАХ ТИПУ $A^{II}B^{IV}$

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Інтеґрал надобмінної взаємодії J_{NN} між магнетними центрами M через немагнетний йон B в напівмагнетних напівпровідниках типу $A^{II}_{1-X}M_XB^{VI}$ досліджено методом алгебри Рака. Як M розглядаються йони Mn^{2+}, Fe^{2+} і Co^{2+}. Враховуються основні орбітальні стани магнетних йонів в кристалічному полі симетрії T_d. Результати розрахунку порівнюються із відомими в літературі експериментальними даними та з результатом експериментальних досліджень ефекту Фарадея в $Cd_{1-x}Fe_xTe$. Показано, що такий підхід дозволяє пояснити зв'язок критичних значень x для систем $Cd_{1-x}Mn_xTe$ та $Cd_{1-x}Fe_xTe$ із величинами інтеґралів J_{NN} для цих систем.