Then

$$m'(k) = \sigma\sqrt{\frac{\pi}{2}}\left(-\frac{k}{\sigma^2} e^{-\frac{k^2}{2\sigma^2}} \sum_{i=0}^{\infty} \frac{(2i+1)!!}{(i!)^2 4^i} \left(\frac{k}{\sigma}\right)^{2i} + \right. \\ \left. + e^{-\frac{k^2}{2\sigma^2}} \sum_{i=0}^{\infty} \frac{(2i+1)!!}{(i!)^2 4^i} \frac{2i \cdot k^{2i-1}}{\sigma^{2i}} \right), \quad (19)$$

$$D\hat{k} = \frac{\sigma^2}{\left(m'(k)\right)^2 N \cdot L}, \quad (20)$$

$$k_{-} = k - 3\sqrt{D\hat{k}}, \quad (21)$$

$$k_{+} = k + 3\sqrt{D\hat{k}}. \quad (22)$$

Fig. 3 shows the curves 4 and 5 corresponding to the curves of noise immunity at k_{-} and k_{+}, respectively. In this case $D\hat{k} = 1.2 \cdot 10^{-19}$, $k_{-} = 6.99999988 \cdot 10^{-1}$ and $k_{+} = 6{,}99999989 \cdot 10^{-1}$. As it is evident from these curves, a decrease in immunity ISPR is observed.

The invariant non-coherent system of information transmission is offered and its qualitative characteristics in conditions of inaccurate definition of thresholds are defined.

The developed method can find application in the systems of information processing.

In the author's opinion it is necessary to compare the noise immunity of the investigated invariant system with the noise immunity of similar invariant systems. That will be done in the subsequent papers.

References

1. Gonorovsky I. S. Radio Engineering circuits and signals M. : Sovetskoye Radio, 1971.

2. Invariant method of analysis of telecommunication systems of information transmission : monograph / V. B. Malinkin, E. I. Algazin, D. N. Levin, V. N. Popantonopulo. 2006.

3. Teplov N. L. The noise immunity of the systems of discrete information transmission. 1964.

4. Levin B. R. Theoretical foundation of statistic radio engineering. The third edition. M. : Radio and communication, 1989.

S. S. Aplesnin, A. I. Moskvin
Siberian State Aerospace University named after academician M. F. Reshetnev, Russia, Krasnoyarsk

MAGNETOELECTRIC EFFECT INDUCED BY ORBITAL ORDERING OF ELECTRONS

Relationship between orbital order and the formation of the spontaneous magnetic moment, lattice constant, correlation function of orbital and spin moments between nearest neighbors have been investigated in terms of the continuous Potts model for set of electron-phonon parameters and spin-phonon interactions. A change in the permittivity and orbital correlation functions in the external magnetic field has been found.

Keywords: permittivity, magnetoelectric effect, electron-lattice interaction, orbital and spin moment.

The study of multiferroics with the coexistence of at least two of the three order parameters (magnetic, electric, and crystallographic) [1] is an urgent problem, for it describes the possibility of controlling the magnetic properties of a material by means of an electric-field and, vice versa, magnetic-field modulation of electric properties. In the future, multiferroics may find wide technical application in sensors and recording devices, reading and storing information. While the spintronic devices transform information by changing the magnetization to electric voltage; in multiferroics the correlation between the magnetic and electric subsystems manifests itself in the magnetoelectric effect [2; 3].

The $Co_xMn_{1-x}S$ solid solutions can be attributed to the multiferroic class [4]. In the temperature ranges of $T \approx 110$–120 K and $T \approx 230$–260 K, the correlation between the magnetic and electric subsystems has been found [5]. The presence of this correlation is confirmed by sharp rise of the magnetization and the maximum in the relative variation of permittivity, measured in the external magnetic field and without it at a lowering temperature [6].

Electron density redistribution inside a 3d-shell arising from electron transitions from e_g to t_{2g} levels; or due to the different electro negativities of cobalt and manganese ions can lead to changes the orbital occupancy at the t_{2g} shell of Mn ions.

An important feature is that magnetic exchange interaction depends on orbital occupancy. This means that even the sign could change. Therefore, it is possible that magnetic correlation at normal can be very different from that in the ordered phase, when the orbital order is accompanied by magnetic transition. The variation of the orbital occupancy may be caused shift in polarizability and in spin state of cation.

The aim of this study is to investigate the physical properties of the $Co_xMn_{1-x}S$ solid solutions typical of multiferroics, induced by spin-charge ordering, and to establish the interrelation between the magnetic, electric, and elastic subsystems.

Interrelation model between electron and elastic subsystems. Interpretation of the results obtained requires consideration of the interrelation between the electron and crystal structures. We shall consider competition between the Coulomb and direct exchange interactions between manganese ions. The consideration of the electrons' kinetic energy induces redistribution of the electronic density between the e_g and t_{2g} levels towards the increase in electron population in the t_{2g} state. In this case, one of the t_{2g} orbitals contains two electrons and hopping between the neighboring sites and different orbitals occurs with no change in the Coulomb interactions of electrons. In addition, kinetic energy of electrons grows due to the formation of a narrow miniband by electron hopping over to the nearest manganese ions in the vicinity of the Fermi level.

For a pair of manganese ions with the half-filled orbitals the integral of electron hopping over sulfur anions can be estimated as $t^x_{\alpha\beta} = E_{x,\alpha}E_{x,\beta}/[(\varepsilon_p - \varepsilon_d) + U]$, where $E_{x,a}$ are the integrals of overlap of the sulfur p-orbitals and manganese t_{2g}-orbitals with the value $E_{x,a}$ = 1.1 eV, $\varepsilon_p - \varepsilon_d$ = 1.5 eV is the charge gap, and U = 4 eV. For two electrons at one of the five d-levels of manganese ions surrounded by sulfur ions, the overlap integral is zero, ($E_{x,a}$ = 0) in virtue of the Pauli principle and upon the lateral oscillations of sulfur ions weak overlap of the electron wave functions of manganese ions with the miniband width of $W = 2zt$ = 0.5 – 0.8 eV is possible. In other words, the transport properties are related to hole hopping over the e_g-orbitals and motion of electrons over the t_{2g}-states. The type of the carriers corresponds to the lattice polarons, i. e., the motion of electrons in the lattice induces the coupled lateral and longitudinal oscillations of sulfur ions and is implemented along one of the subbands of the t_{2g} band with the orbital magnetic moment, while in the e_g band motion of the current carriers is directly connected with the type of the magnetic structure. As a result, different population of the *dxy*-, *dxz*-, and *dyz*-orbitals is induced and orbital-charge ordering forms accompanied by ordering the orbital angular moments.

In the phenomenological representation, the Hamiltonian for two orbitals x and y and two sites can be written as:

$$H = -J_1(n_{1x} - n_{1y})(n_{2x} - n_{2y})(1-c) - g(n_{1x} + n_{2x})(1-c)x -$$
$$- g(n_{1y} + n_{2y})(1-c)y + \frac{1}{2}k(x^2 + y^2) - b(x^3 + y^3) -$$
$$- h(n_{1x} + n_{2x} - n_{1y} - n_{2y})(1-c) - J_2(n_{1ix} - n_{1iy})(n_{2ix} - n_{2iy})c -$$
$$- KM_1M_2 - g_s(x+y)M_1M_2 - \lambda(1-c)\left(n_{1x} - n_{1y}\right)M_1 -$$
$$- \lambda(1-c)(n_{2x} - n_{2y})M_2 - h(M_1 + M_2) - h(n_{1ix} - n_{1iy} +$$
$$+ n_{2ix} - n_{2iy})c - c\lambda\left(n_{1ix} - n_{1iy}\right)M_1 - \lambda\left(n_{2ix} - n_{2iy}\right)M_2c,$$

where $n_{1,2ix}$ and $n_{1,2x,y}$ are the electron densities on the *dxz*- and *dyz*-orbitals of manganese ions surrounding a cobalt ion with concentration c and on manganese ions in the matrix with concentration (1 – c), J_1 and J_2 are the exchange interactions between the orbital magnetic moments Mn–Mn and Co-Mn, g is the parameter of the electron-lattice interaction, x and y are the displacements of ions in the directions corresponding to the square sides, k and b are the elastic constants, h is the magnetic field, a is the lattice constant, $K < 0$ is the exchange interaction between magnetic moments M_1 and M_2, g_s is the constant of the spin-lattice interaction, and λ is the parameter of the spin-orbital coupling. At the interaction of orbital and spin moments, the high-order terms (L_1L_2) (M_1M_2) appear, but for the t_{2g} electrons they are much smaller than the spin-orbital interaction.

Now, within this Hamiltonian, we will try to answer a number of questions. How do the concentration of the Mn-Co-Mn clusters and the effective orbital interaction influence the temperature of the formation of the spontaneous magnetic moment? How will the lattice parameter change at orbital-charge and magnetic ordering? Which changes in the temperature behavior of the orbital correlation functions (correspondingly, charge redistribution) will result from action of the external magnetic field?

The estimate density of the electron on the t_{2g} orbitals of manganese ions in the matrix by the value of the spin moment at site S = 4.4 μ_B for MnS ($n_{1,2}$ ~ 0.1). The electron density in the Mn-Co cluster can reach value $n_{1,2i} \sim 0.5$.

Thermodynamic characteristics of model. We shall calculate the thermodynamic characteristics, the correlation function between the nearest neighbors for the orbital $\langle L_1\ L_2\rangle$ ($L = n_{1x} - n_{1y}$) and magnetic $\langle M_1\ M_2\rangle$ moments, and the average displacement along the OX $\langle x\rangle$ and OУ $\langle y\rangle$ axes using a continuous Potts model, where the quantities vary within intervals $0 < n_{1,2x,y} < 0.1$, $0 < n_{1,2ix} < 0.5$, $0 < x,y < 1$, and $-1 < M_{1,2} < 1$.

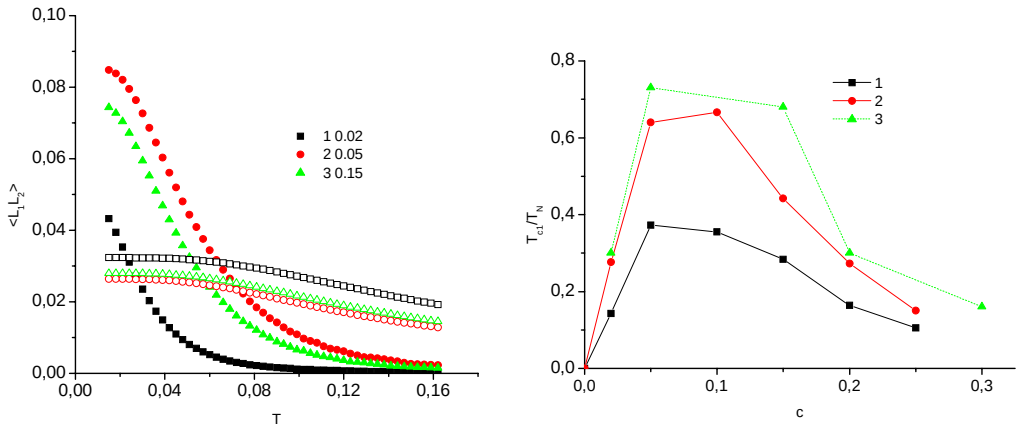
The correlator of the magnetic moments in the region of the transition temperature from the magnetically ordered to paramagnetic phase decreases by a factor of two or three, and has an inflection point. Therefore, we associate the temperature at which the long-range ferromagnetic order of the orbital moments disappears with the temperature at which the inflection in the temperature dependence of the correlation function $\langle L_1\ L_2\rangle$ (T) and $\langle M_1\ M_2\rangle$ (T) is observed. Fig. 1, *a* depicts temperature dependences of the correlators for several concentrations of cobalt ions. One can extract two temperatures T_c and T_{c1} at which the orbital magnetic moments of manganese ions and the orbital moments of the Mn-Co-Mn clusters are ordered. The typical concentration behavior of T_{c1} (c) is presented in fig. 1, *b* for two exchange parameters J_2/J_1. It correlates with the concentration of the Mn-Co-Mn clusters in dependence of cobalt concentration $c = zx\ (1–x)^{z-1}$, where z = 12 is the number of the nearest neighbors for the FCC lattice. According to the results of our calculations, the dependence of T_{c1} from the value of the exchange between the orbital magnetic moments in the Mn-Co-Mn cluster is linear with the slope depending on the concentration of cobalt ions and the electron-lattice interaction which shifts the temperature of the transition of orbital ordering towards the higher temperatures within 20 % with an increase in $g/J \sim 1$. The experimental results illustrated in

Fig. 1 are described satisfactorily within the model with orbital ordering of the angular moments.

Let us now consider the effect of the electron-lattice and spin-lattice interactions on lattice deformation and variation in the lattice constant with temperature. Fig. 2 shows temperature dependences of the average displacement of ions for several parameters of the electron-lattice and spin-lattice interactions with allowance made for unharmonism of the lattice oscillations. The interaction of electrons with allowance for the lattice degrees of freedom leads to the increase in distance between electrons, i. e., to the growth of the lattice constant. In particular, the displacement is directly proportional to the constant of the electron-phonon interaction $\langle x \rangle = gn/k$ in the systems with strong electron correlations, when the Coulomb interaction exceeds the band width and unharmonism of the oscillations is neglected. With an increase in the value of the electron-lattice interaction, the change in the slope is observed at some temperature which shifts towards higher temperatures as g grows.

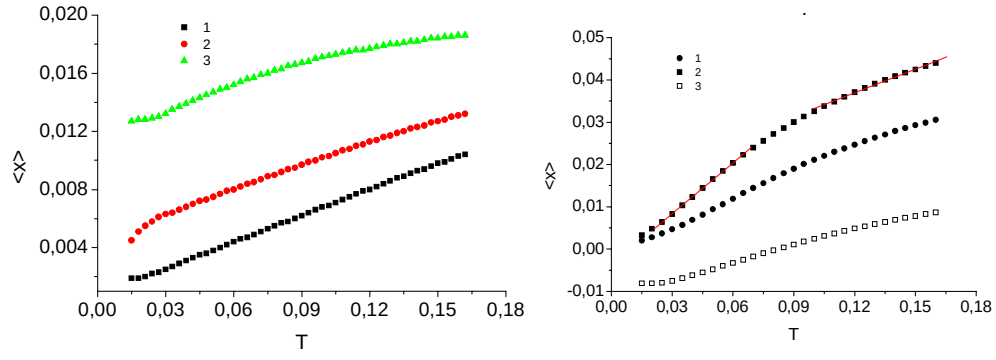
The exchange interaction between the localized spins depends exponentially on the distance; due to the lattice compression the density of overlap of the wave functions grows and the exchange energy increases. The enhancement of the spin-lattice coupling leads to a change in the sign of the average ion displacement. In fig. 2, one can see temperature dependences of $\langle x \rangle$ on two concentrations and two parameters of the spin-lattice coupling. Due to the competition of the electron-lattice and spin-lattice interactions, the lattice compresses. The change in the slope of the dependence $d < x > /dT$ is observed in the region of the transition to the magnetically ordered state.

In the presence of the spin-orbital interaction, fluctuations of the magnetic moments in two sublattices are asymmetric; as a result, the total magnetic moment $M_1 + M_2$ with the maximum at the Neel temperature is induced (fig. 3). This is similar to the action of the external magnetic field $h_{ef} = \lambda \langle L \rangle$, when the magnetization value of one of the sublattices changes. Redistribution of the electron density on the *dxz*- and *dzy*-orbitals results in the occurrence of the tetragonal distortion illustrated in fig. 3 for several parameters of the spin-orbital coupling.



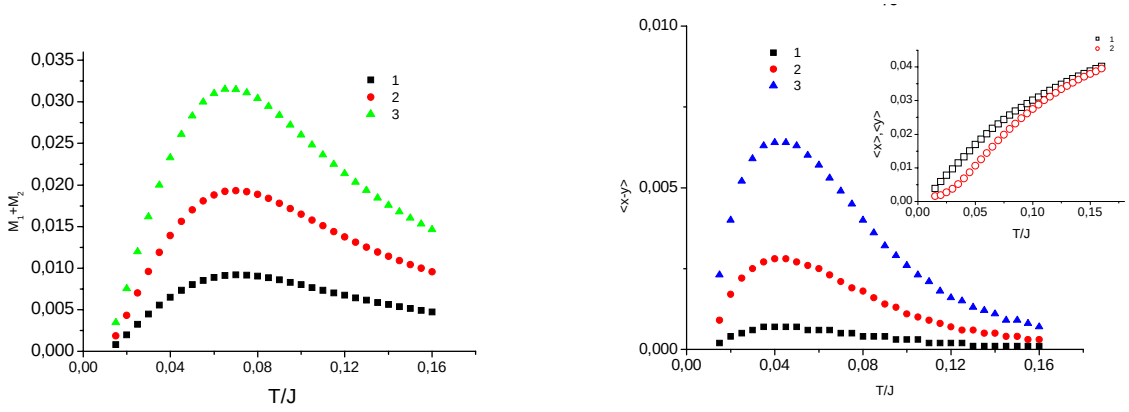
a *b*

Fig. 1. Correlation of magnetic orbital moments $\langle L_1 L_2 \rangle$ (*a*) in the matrix of manganese ions (light symbols) and in the Mn-Co-Mn cluster (dark symbols) versus temperature for the parameters $J_1 = 10$, $J_2 = 6$, $g = 6$, $k = 20$, $b = 3$, $K = -0.35$, $g_s = 0.1$, $\lambda = 0.1$, and $x = 0.02$ (1), 0.05 (2), and 0.15 (3) (*a*). The temperature of the orbital magnetic moment formation in the Mn-Co-Mn cluster is normalized by the Neel temperature for the parameters $J_2 = 5$ (1), 8 (2), $J_1 = 10$, $g = 6$, $k = 20$, $b = 3$, $K = -0.35$, $g_s = 0.1$, and $\lambda = 0$ versus cobalt concentration (*b*)



a *b*

Fig. 2. Average ion displacement $\langle x \rangle$ versus temperature for the parameters of the electron-phonon interaction $g = 2$ (1), 5 (2), and 8 (3) with $b = 1$, $J_2 = 6$, $J_1 = 10$, $k = 20$, $K = -0.35$, $g_s = 0.1$, $\lambda = 0$, and $x = 0.15$ (*a*) and for the two parameters of the spin-phonon interaction $g_s = 0.1$, $x = 0.02$ (1), $x = 0.05$ (2), $g_s = 0.2$, and $x = 0.05$ (3) with $J_1 = 10$, $J_2 = 6$, $g = 6$, $k = 20$, $b = 3$, $K = -0.35$, and $\lambda = 0.1$ (*b*)



a *b*

Fig. 3. Total magnetization ($M_1 + M_2$) of the spin moments (*a*) and tetragonal distortion <*x*–*y*> of the lattice (*b*) versus temperature for the parameters of the spin-orbital interaction $\lambda = 0.1$ (1), 0.2 (2), and 0.3 (3) with $J_1 = 10$, $J_2 = 5$, $g = 6$, $k = 20$, $b = 3$, $K = -0.35$, $g_s = 0.1$, and $x = 0.05$. The insert shows the temperature dependence of lattice parameters <*x*> (1) and <y> (2) for $\lambda = 0.3$

The change in the electron density at e_g and t_{2g} states induces electron polarization of an ion determined by the polarizability of an atom $\alpha = \alpha_n + 2b_n\,[M^2_J - 1/3\,J(J+1)]$, where α_n and b_n are the constants, J is the total moment of an atom, M_J is the projection of the moment onto a selected direction. Permittivity is related to polarizability as $\varepsilon = 1 + 4\pi N\alpha$ and the change in permittivity in the external magnetic and electric fields is determined as $\Delta\varepsilon \sim \Delta\alpha \sim \Delta\, M^2_J \sim \Delta < L_1L_2 >$. Reconstruction of orbital structure by the magnetic or electric fields will manifest itself in the variation of the correlation functions. In fig. 4, one can see the difference in the correlators of the orbital magnetic moments calculated with and without the magnetic field for several concentrations.

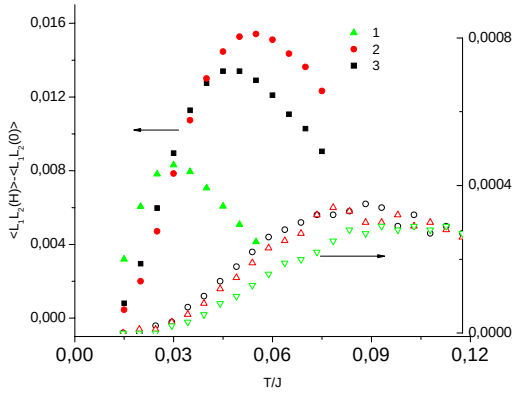


Fig. 4. Difference between the correlation functions of the orbital magnetic moments for the Mn-Co-Mn clusters (left scale) and manganese ions (right scale) calculated with and without magnetic field versus temperature for $J_1 = 10$, $J_2 = 5$, $g = 6$, $k = 20$, $b = 3$, $K = -0.35$, $g_s = 0.1$, $\lambda = 0.1$, and $x = 0.02$ (1), 0.05 (2), and 0.15 (3)

The first maximum in the low-temperature region is caused by the change in the orbital correlation function in the Mn-Co cluster; the second maximum is related to the growth of the orbital order in the manganese system. This qualitatively explains the presence of two maxima in the ME effect. A similar behavior is observed in the external electric field due to the change in the electron density on the orbitals caused by the dependence on the potential energy of an electron at a distance in the external uniform electric field. The substantial contribution to permittivity is made also by the Jan-Teller ion displacement, which is not considered in this model.

The competition of the Coulomb interactions between the electrons located on one orbital and on different orbitals along with the change in the hopping integrals causes ordering the electrons on the certain orbitals and orbital magnetism. Due to the redistribution of the electron density, the elastic energy changes and coupled modes of the ion oscillations are induced under the action of the electron-phonon interaction. The magnetoelectric effect magnitude is estimated.

References

1. Epitaxial $BiFeO_3$ Multiferroic Thin Film Heterostructures / J. Wang [et al.] // Science. 2003. Vol. 209. P. 1719–1728.

2. Zvesdin A. K., Pyatakov A. P. Phase transition and colossal magnetoelectric effect // UFN. 2004. Vol. 174. P. 465–468.

3. Smirnov A. I., Hlusticov I. N. Magnetoelectric effect and Stark effect // UFN. 1995. Vol. 165. P. 1215–1219.

4. Transport Properties and Ferromagnetism of $Co_xMn_{1-x}S$ Sulfides / S. S. Aplesnin [et al.] // JETF. 2008. Vol. 106, № 4. P. 765–772.

5. Magnetoelectric effect in $Co_xMn_{1-x}S$ / S. S. Aplesnin [et al.] // Vestnic of SibSAU. 2009. Vol. 1(22). P. 41–45.

6. Spin Glass Effects in $Co_xMn_{1-x}S$ Solid Solutions / S. S. Aplesnin [et al.] // Bulletin of the Russian Academy of Sciences: Physics. 2009. Vol. 73, № 7. P. 965–967.