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The phase-separated states in antiferromagnetic semiconductors with polarizable lattice

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Abstract

The possibility of the slab or stripe phase separation (alternating ferromagnetic highly-conductive and insulating antiferromagnetic layers) is proved for isotropic degenerate antiferromagnetic semiconductors. This type of phase separation competes with the droplet phase separation (ferromagnetic droplets in the antiferromagnetic host or vice versa). The interaction of electrons with optical phonons alone cannot cause phase-separated state with alternating highly-conductive and insulating regions but it stabilizes the magnetic phase separation. The magnetostriction deformation of the lattice in the phase-separated state is investigated.

1 Introduction

In magnetic semiconductors there are two main mechanisms of the charge carrier self-trapping: magnetic and polaronic. The former corresponds to trapping of the electron by a microregion of a changed magnetic phase created by this electron. This effect is most energetically favored in antiferromagnetic semiconductors where the self-trapping occurs in ferromagnetic microregions. On the other hand, the magnetic semiconductors are partly polar crystals. For this reason polaronic effects should exist in them. The electron-phonon interaction is not so strong in them as in the completely polar NaCl-type crystals, and only it alone cannot change the state of the charge carriers drastically. In particular, the small polarons are impossible in the magnetic semiconductors. Otherwise, they would not be degenerate at heavy dopings, and the charge carriers would not realize the indirect exchange in them. But, being added to the magnetic mechanism of the self-trapping, the lattice mechanism can considerably increase the stability of the self-trapped state.

In degenerate antiferromagnetic semiconductors the magnetic self-trapping is a cooperative phenomenon. It manifests itself as a phase separation into the highly-conductive ferromagnetic phase and insulating phase as a
result of the fact that all the charge carriers concentrate inside the ferromagnetic phase\textsuperscript{5,6}. Both these phases are charged oppositely. Due to the Coulomb interaction between them the phase intermixing takes place.

Two main types of such intermixing were considered in an isotropic crystal: the droplet one\textsuperscript{6} and the slab one\textsuperscript{5}. In the former case at relatively low charge carrier densities, droplets of a metallic ferromagnetic phase arise inside an insulating antiferromagnetic host, with all the charge carriers concentrated inside these droplets. At larger densities, the highly-conductive ferromagnetic phase occupies the larger part of the volume, and the antiferromagnetic phase is represented by insulating droplets inside it. The slab structure corresponds to alternating highly-conductive ferromagnetic and insulating antiferromagnetic plane layers. As a particular case, it includes the stripe structure with the ferromagnetic phase consisting of monolayers which separate the antiferromagnetic slabs. As is well known, the stripe structure attracts much attention in connection with the manganites, nickelates, and high $T_c$ superconductors nowadays.

In the pioneering paper [5] only very crude estimates of the energy of the slab phase-separated state were carried out. The electric properties of such a phase-separated state should be highly anisotropic: it should be highly-conductive along the layers and insulating across them for any charge carrier density in the range where the phase separation is realized. In the subsequent paper [6] much more accurate calculations were carried for the droplet model. This model made it possible to explain the transition from the insulating state to the highly-conductive state with increasing charge carrier density as a result of the percolation of the ferro-electronic liquid, i.e. of changing the topology of the ferromagnetic phase from multiply-connected to simply-connected. Such a transition was observed experimentally in EuSe and in other materials (see Refs. [3,7]).

The problem of the phase separation becomes again highly actual due to enhanced interest to the manganites. The coexistence of the ferromagnetic and antiferromagnetic phases in them was established very long ago\textsuperscript{8}. There are new experimental data which evidence coexistence of these types of the magnetic ordering (e.g., Refs. [9-16]). Though sometimes these data were interpreted in terms of the canted antiferromagnetic ordering, one should keep in mind that it is unstable against fluctuations of the charge carrier density\textsuperscript{3,17–21}. For this reason one can assume that these properties are related to the ferro-antiferromagnetic phase separation. This makes it necessary to reinvestigate theoretically the phase separation in the degenerate antiferromagnetic semiconductors more accurately. In particular, it is nec-
cessary to find out whether the slab structure is really impossible in them.

The present paper is devoted to this problem. A more general model than in Refs. [5,6] is used here which takes into account not only the magnetic self-trapping but also the polarization that. For this reason essentially new results are obtained not only for the slab structures but also for the droplet ones. It will be shown that for some systems, both polarizable and nonpolarizable, the difference in the energies of the slab and droplet structures is so small that it is below the accuracy of the calculation. Hence, one cannot state with certainty that the slab structure is impossible in the isotropic antiferromagnetic crystals. The small difference in the energies assumes that a small force can transform one structure into the other even if the latter is normally unstable. For example, if normally the droplet structure is stable, a small uniaxial deformation can stabilize the slab structure.

Independently of the type of the structure, the lattice polaronic effects can essentially influence the electron-magnetic phase separation making it considerably more stable. They increase the size of the ferromagnetic regions in both droplet and slab structures. On the other hand, they increase the density of electrons in the ferromagnetic phase. As a result, the total volume of the ferromagnetic phase and the total magnetization of the crystal become decreased. Hence, the electron-lattice interaction, suppressing the ferromagnetic phase, hinders the metal-insulator transition for the droplet geometry and the transition to the uniform ferromagnetic state for both geometries.

Especially large is contribution of the polaronic effect in the case when the polaronic attraction between the charge carriers almost compensates the Coulomb interaction arising due to the mutual charging of both phases. If the former exceeds the latter, the phase separation of the types discussed here becomes impossible. The condition for this the inequality \( \frac{\epsilon_0}{2} < \epsilon_\infty \), where \( \epsilon_0 \) and \( \epsilon_\infty \) are the static and high-frequency dielectric constants, respectively. But such a situation will not be considered here. There are antiferromagnetic semiconductors, in which \( \epsilon_0/2 \) only slightly exceeds \( \epsilon_\infty \), e.g., EuSe with \( \epsilon_0 = 9.4 \) and \( \epsilon_\infty = 5.0 \) [22], so that the investigation of the polaronic effects close the stability boundary is a quite actual problem.

Recently some authors expressed the point of view that the purely polaronic phase separation is possible in the manganites without magnetic phase separation (e.g., [23]). This seems hardly possible as such a state would correspond to formation of regions consisting of the Pekar polarons. But, as is well known, the Pekar polarons are impossible for realistic parameter values. This qualitative consideration was confirmed numerically using the
procedure described below. The situation can be different when the small polarons are more energetically favored than the large polarons. According to Ref. [24], the small polaron condensation into a string is possible. But, as was already mentioned, the small polarons do not exist in the magnetic semiconductors.

It should be noted that other types of the electron-phonon interaction can be essential for certain systems. In Ref. [25] the idea was advanced that the interaction between the electrons and Jahn-Teller phonons can cause the phase separation in the manganites. But this problem will not discussed here. In Ref. [26] the magnetostriction at the magnetic single-electron self-trapping was investigated. In the present paper the modulation of the lattice due to the interaction of the slab structure with the acoustical phonons will be investigated. The problem of magnetostriction at the electron self-trapping became actual now due to its experimental discovery [27, 28].

2 The Hamiltonian of the system

The Hamiltonian of the system consists of the Hamiltonian of the $s-d-$model $H_{sd}$, the free phonon Hamiltonian $H_p$ and the Hamiltonian $H_{sp}$ of the $s$-electron-phonon interaction.

\[
H = H_{sd} + H_{sp} + H_p + H_C \tag{1}
\]

\[
H_{sd} = t \sum a_{g,\sigma}^* a_{g+\Delta,\sigma} - A \sum (s_S)_\sigma (a_{g\sigma}^* a_{g'\sigma}) - \frac{I}{2} \sum S_g S_{g+\Delta} \tag{2}
\]

where $a_{g\sigma}^* , a_{g+\Delta\sigma}$ are the $s$-electron operators, corresponding to the conduction electrons or holes at the atom $g$ with the spin projection $\sigma$, $s$ is the $s$-spin operator, $S_g$ that of the $d$-spin of the atom $g$, $\Delta$ the vector connecting the first nearest neighbors. The crystalline structure is assumed to be simple cubic, the $d$-spin magnitude being $S$. As usually, the inequality $t \gg IS^2$ must be met as the hopping integral $t$ is of the first order of magnitude, and the $d-d-$ exchange integral $I$ of the second order in the small $d-$ orbital overlapping.

The free phonon Hamiltonian for essential phonons is given by the standard expression

\[
H_p = \sum \omega_q b_q^\dagger b_q \quad (\hbar = 1) \tag{3}
\]
where $b_q^* b_q$ are the operators of the phonons with the wave vector $q$.

The electron-phonon Hamiltonian can be presented in the form

$$H_{sp} = - \sum [C_q \exp(iq\mathbf{g}) b_q a_{g\sigma}^* a_{g\sigma} + \text{H.C.}] \quad (4)$$

In the long-wave approximation, the interaction constant with the longitudinal optical phonons is given by the expression

$$C_q^a = -ie \sqrt{2 \pi \omega / \epsilon \epsilon_0 V q}, \quad \frac{1}{\epsilon^*} = \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \quad (5a)$$

where $\omega$ is the longitudinal optical phonon frequency, $V = Na^3$ is the volume of the crystal, $a$ is the lattice constant. For the longitudinal acoustical phonons in the deformation potential approximation the electron-phonon constant is

$$C_q^a = i E_1 q \sqrt{\frac{k^2}{2\omega \omega MN}}, \quad \omega = sq \quad (5b)$$

where $E_1$ is the deformation potential constant, $M$ the mass of the unit cell.

The term $H_C$ describes the Coulomb energy of interaction of the $s$-electrons with each other and with ionized impurities. The charge of the latter compensating the charge of the charge carriers is assumed to be distributed uniformly over the sample (the jellium model).

## 3 The variational procedure

The reason for the magnetoelectronic phase separation in an antiferromagnetic semiconductor is the fact that the charge carrier energy is lower for the ferromagnetic ordering than for the antiferromagnetic that. If the charge carrier density is insufficient to make the entire crystal ferromagnetic, the charge carriers can concentrate in a portion of the crystal and make it ferromagnetic.

Obviously, the ferromagnetic and antiferromagnetic phases are charged oppositely. To diminish the Coulomb energy, these phases should intermix. Two geometries will be considered. The first of them assumes that a crystal becomes separated into alternating layers of a highly-conductive ferromagnetic phase and the insulating antiferromagnetic phase. The second is the droplet geometry of the phase separated state investigated in Ref. [6]. Only
the charge carrier densities below the percolation threshold will be considered here which corresponds to the ferromagnetic highly-conductive droplets inside the antiferromagnetic host.

Like in Refs [5,6], a variational procedure will be used here to find the ground-state energy of the phase-separated system. One of the variational parameters is the ratio of the volume of the antiferromagnetic phase to that of the ferromagnetic phase $X$. For the slab geometry the second variational parameter is the thickness of the ferromagnetic layers $L$ with the antiferromagnetic layers of a thickness $XL$ (in the lattice constants $a$). Both numbers $L$ and $XL$ are assumed to be integer. Then, if the lattice is simple cubic, the electrons are concentrated in the ferromagnetic layers with dimensionless coordinates $f_x = nL(1 + X) + g_x, (1 \leq g_x \leq L)$ where their number per atom $\nu(x)$ is equal to $\nu_0(1 + X)$ ($\nu_0$ is the mean number of $s$-electrons per magnetic atom, $n$ an integer). Outside these layers the number of the conduction electrons is zero. For the droplet geometry the second variational parameter is the radius of the ferromagnetic droplet $R$.

In the ferromagnetic phase all the charge carriers are assumed to be spin-polarized. For $W = 12t \ll AS$ this condition is met for all the charge carrier densities. For $W = 12t \gg AS$ it is met when $AS > \mu$ where $\mu$ is their Fermi energy.

Two approaches will be considered here. The first one, sketched in Ref. [5] and used in Ref [6], is valid for large $L$ or $R$. In this case, in addition to the standard bulk kinetic energy $E_B$, the surface electron energy $E_S$ must be introduced which stems from spatial quantization of the electron levels. Just competition of the surface energy and the Coulomb energy ensures a finite size of the ferromagnetic regions. The second approach assumes that a $s$-electron is confined to a single atomic plane, i.e., that its motion is two-dimensional ($L = 1$). The ground-state total energy of the phase-separated system $E_{PS}$ (per unit cell) can be represented in the form:

$$E_{PS} = E_k - \frac{AS\nu_0}{2} + E_C + E_{dd} + E_{pol}$$

(6)

For large $L$ or $R$, the kinetic energy of the system can be presented in the form

$$E_k = E_B + E_S$$

(7)

Here the bulk kinetic energy of the charge carriers $E_B$ is given by the expression valid for relatively small $\nu$:

$$E_B = -6t\nu_0 + K(1+X)^{2/3}, \quad K = 0.6\mu(\nu_0)\nu_0, \quad \mu(\nu) = t(6\pi^2\nu)^{2/3}$$

(8)
where \( \nu_0 \) is the mean s-electron number per unit cell.

The term \( E_S \) is the surface energy of the electron gas. Like in Ref. [6], it is calculated in the Born-Oppenheimer approximation, i.e. by expansion in \( 1/[\nu_0 L(1+X)] \) powers. The Dirichlet boundary conditions for the s-electron wave function are taken. For the slab structure

\[
E_S^s = \frac{2^{2/3}5\pi^{1/3}K(1+X)^{1/3}}{3^{1/3}16\nu_0^{1/3}L} \quad (9a)
\]

and for the droplet structure

\[
E_S^d = \left(\frac{\pi}{6}\right)^{1/3} \frac{15K}{16\nu_0^{1/3}(1+X)^{1/3}R} \quad (9b)
\]

For the case of \( L = 1 \) one obtains the following expression for the total kinetic energy

\[
E_k^1 = -4t\nu_0 + 2\pi\nu_0^2(1+X)t \quad (10)
\]

The term \( E_C \) in Eq (6) representing the Coulomb energy of the phase- and charge-separated state is calculated using the jellium model: the total compensating charge with the density \(-e\nu_0\) modeling the charge of ionized donors or acceptors is distributed uniformly over the crystal. For the slab structure one has:

\[
E_C^s = \frac{\pi e^2\nu_0^2L^2X^2}{6\epsilon_0a} \quad (11a)
\]

For the droplet structure the calculation is carried using the Wigner spheres of a radius \( R_W \) surrounding the ferromagnetic droplets. The total charge of the Wigner sphere is zero so that \( R_W = R(1+X)^{1/3} \). Hence,

\[
E_C^d = \frac{2\pi e^2\nu_0^2R^2[2X + 3 - 3(1+X)^{2/3}]}{5\epsilon_0a} \quad (11b)
\]

The change in the \( d-d \)-exchange energy due to the formation of the ferromagnetic regions is given by

\[
E_{dd} = \frac{D}{1 + X}, \quad D = -zIS^2 \quad (12)
\]

where \( z = 6 \) is the coordination number for a simple cubic lattice, \( I < 0 \).
4 The polaronic energy

The polaronic energy \( E_{pol} \) entering Eq. (6) is found from the effective lattice Hamiltonian \( H_{pol} = H_p + \langle H_{sp} \rangle \) where the symbol \( \langle ... \rangle \) denotes averaging over the ground state of the electronic-magnetic subsystem. This corresponds to the adiabatic approximation in the polaron theory which is justified even for a weak electron-phonon coupling since the nonuniform electron distribution arises not due to the phonons in a selfconsistent manner but due to the magnetization. This distribution is given in advance with respect to the phonons.

For the slab structure one obtains from Eq. (4):

\[
\langle H_{sp} \rangle = - \sum_{\mathbf{r}, \mathbf{q}} C_\mathbf{q} \nu(f_x)[b_{\mathbf{q}} \exp(i\mathbf{qf}) + \text{H.C.}],
\]

\[
\nu(f_x) = \nu_0(1 + X) \sum_n \Theta[f_x - n(1 + X)L] \Theta[n(1 + X)L + L - f_x],
\]

where \( \Theta(z) = 1 \) for \( z > 0 \) and \( \Theta(z) = 0 \) for \( z \leq 0 \).

One obtains from Eqs (13), (14):

\[
\langle H_{sp} \rangle = -iN_y N_z \nu_0(1 + X) \sum_{\mathbf{q}_x} C(\mathbf{q}_x, 0, 0) b_{\mathbf{q}_x, 0, 0} \mathcal{P}(\mathbf{q}_x) \mathcal{P}(\mathbf{q}_x) + \text{H.C.},
\]

\[
\mathcal{P}(\mathbf{q}_x) = \frac{\exp(i\mathbf{q}_x L) - 1}{\exp(i\mathbf{q}_x) - 1},
\]

\[
\mathcal{P}(\mathbf{q}_x) = \frac{\exp[iq_x GL(1 + x)] - 1}{\exp[iq_x L(1 + x)] - 1},
\]

where

\[
G = \frac{N_x}{L(1 + X)}
\]

is the number of pairs of the ferromagnetic and antiferromagnetic layers, \( L(1 + X) \) the dimensionless thickness of a pair of these layers. As \( G \to \infty \), the quantity \( \mathcal{P}(\mathbf{q}_x) \) is nonzero only for \( q_m = 2\pi m/[a(1 + X)L] \) where \( m \) is an integer. Hence,

\[
\mathcal{P}(\mathbf{q}_x) = G \sum_{m=-Y}^{Z} \delta \left( q_x a, \frac{2\pi m}{(1 + X)L} \right),
\]

\[
Y = \frac{L(1 + M)}{2} + \frac{1}{4}[\cos(\pi(1 + X)L) - 1]; \quad Z = Y - 1
\]
where $\delta(n,m) = 1$ for $n = m$ and 0 otherwise.

Using Eqs (16), (17) and diagonalizing the averaged phonon Hamiltonian $H_{pol}$ (3), (13 - 15) by the well known procedure of the phonon operator shift

$$b_m \rightarrow b_m + \beta_m, \quad \beta_m = \frac{N\nu_0 C_m p(q_m)}{L\omega_m}, \quad (20)$$

$$m = \left( \frac{2\pi m}{a(1 + X)L}, 0, 0 \right), \quad N = N_x N_y N_z$$

one obtains the following expression for the cooperative polaron energy per unit cell:

$$E_{pol} = -\frac{N\nu_0^2}{L^2} \sum_{m=-Y}^{Z} \frac{|C_m|^2 |p(q_m)|^2}{\omega_m}, \quad (21)$$

$$|p(q_m)|^2 = \frac{1 - \cos 2\pi m / (1 + X)}{1 - \cos 2\pi m / [(1 + X)L]}$$

The term with $m = 0$ is omitted from Eq (21) as it is compensated by interaction of phonons with the ionized impurity charge.

For the droplets such an accurate calculation of $E_{pol}$ will not be carried out for a reason pointed out in the end of this Section. It is sufficient to evaluate this quantity again using the approach based on the Wigner spheres. Then in the adiabatic approximation (e.g., Ref. [3])

$$E_{pol}^d = -\frac{1}{8\pi \epsilon^*} \int D^2(r) d^3r \quad (22)$$

where $D(r)$ is the electric induction. Calculating this quantity for each Wigner sphere and multiplying it by their number, one comes to the expression for $E_{pol}^d$.

To determine $E_{pol}^s$ using the same simplified treatment, one should note that one can introduce an analogue of the Wigner spheres for the slab structure, too. Namely, one can introduce the Wigner layers with the total zero charge, consisting of the highly-conductive layer with the $x$ coordinates between $-L/2$ and $L/2$ and two adjacent insulating half-layers between $L(1 + X)/2$ and $L/2$ and symmetrical one. For them in the adiabatic approximation (22) one arrives to an expression for $E_{pol}^s$ similar to that for $E_{pol}^d$. For them both

$$E_p = -E_{pol}^s \epsilon \quad (23)$$
The question arises about the accuracy of Eq (23). One observes that for the slabs one obtains the same expression directly from Eqs (21), (11a) if the quantities $L$ and $X$ tend to $\infty$ and to 0, respectively. The same occurs for any $L$ as $X \to \infty$. Really, in this case the sum over $m$ in Eq (21) becomes equal to $2X^2L^2\zeta(2)$ where $\zeta(n)$ is the Riemann zeta-function. Hence, Eq (23) and its analogue are valid for large-scale phase separation with relatively small increase in the density or for very large volumes of the antiferromagnetic phase independently of the size of the ferromagnetic layers. As follows from Eqs (11a,b) and (23), the polaron instability ($E_C + E_p < 0$) should occur for

$$\frac{\epsilon_0}{2} < \epsilon_\infty \quad (24)$$

If these conditions are not met, Eqs. (21) and (23) lead to different results. For example, if one takes $\epsilon_0 = 5$ and $\epsilon_\infty = 2.5$, then one obtains by numerical calculations from Eqs (21) and (11.a): $E_p/E_C = 1.0008$ for $L = 1$ and $k \equiv XL = 1000$ or for $L = 1000$ and $k = 1$ in agreement with Eq (23). But for $L = k = 1$ one obtains a value of 2.4317 for this ratio. This means that for such a structure the polaronic effects are considerably stronger than for thicker ferromagnetic or antiferromagnetic layers. Hence, in principle, they can stabilize the stripe structure when the ferromagnetic layers are reduced to monoatomic planes (the long-rang ferromagnetic ordering is possible in the two-dimensional systems even at $T \neq 0$ due to the magnetic anisotropy).

As is seen from Eqs (23) and (11a,b), in the adiabatic approximation used here the polaronic energy vanishes for the uniform ferromagnetic state (for the slab structure it follows from the fact that according to Eq (21) $p(q_m) = 0$ for $X = 0$).

Now we return to the problem of a calculation of the polaronic energy in the manner similar to that leading to Eq. (21). As follows from above-said, such a calculation could be very useful for monoatomic sublattices which are the limiting case for the droplet model. But such sublattices have nothing in common with the phase separation as single atoms cannot form a ferromagnetic phase. Thus, this problem is beyond the framework of the present paper, and for this reason is not considered here. The Eq. (23) is sufficient for the droplet model which assumes that the size of the ferromagnetic droplets is large compared with the lattice constant.
5 Calculations and their results

Now results of calculations will be presented. First, it should be noted that a necessary condition for a phase-separated state to be energetically favored consists in the requirement that the energy (6) be less than the energy of the uniform antiferromagnetic state $E_{AF}$:

$$E_{AF} = -6t\nu_0 + 2^{-2/3}K \quad \text{for} \quad W \gg AS$$  \quad (25)

$$E^{de}_{AF} = -\frac{6t\nu_0}{\sqrt{2S + 1}} + \frac{K}{\sqrt{2S + 1}} - \frac{AS\nu_0}{2} \quad \text{for} \quad W \ll AS$$  \quad (26)

The latter Equation for the double-exchange system is obtained using an expression for the charge carrier energy in a system with the double exchange, if the $d$-spins are quantum [3]. It should be noted that the term $AS/2$ does not disappear for any type of the magnetic ordering playing the part of an additive constant in the case of the double exchange.

According to Eq (23), if one wishes to account for the polaronic effects, in the case of sufficiently large radii $R$ or layer thicknesses $L$ one can introduce the effective dielectric constant $\kappa$, defined by the relationship

$$\frac{1}{\kappa} = \frac{1}{\epsilon_0} - \frac{1}{\epsilon^*} = \frac{1}{\epsilon_0} - \frac{2}{\epsilon_\infty}$$  \quad (27)

In this case one can carry out the minimization of the energies (6-9a,b),(11a,b),(12) with respect to $R$ or $L$ in an explicit form, and then only the minimization with respect to $X$ should be carried numerically. If one interested only in the pure magnetic self-trapping, one should leave Eqs (11a,b) as they stand, and if one wishes to take into account the polaronic contribution, one should replace $\epsilon_0$ by $\kappa$ (27) in them.

In this case one can exclude the quantities $R$ or $L$ from the expressions (6) for the energy and make it a function of the only variational parameter $X$. For the droplets structure with both ferromagnetic and antiferromagnetic droplets this procedure was carried out in Ref. [6]. For the slab structure this program was not carried out yet.

For the droplet model, as in Eq (6) only the terms $E^d_S$ and $E^d_C$ are $R$-dependent, one should replace the sum $E^d_S + E^d_C$ by its minimal value with respect to $R$:

$$E^d_{SC} \approx 1.2\nu_0\gamma[2X + 3 - 3(1 + X)^{2/3}]^{1/3}(1 + X)^{2/9}$$  \quad (28)
\[ \gamma = \left[ \frac{\mu(\nu_0)^2 e^2 \nu_0^{1/3}}{\epsilon_0 a} \right]^{1/3} \]

and substitute the following expression for the radius:

\[ R = \left\{ \frac{75K(1 + X)^{1/3}\epsilon_0 a}{6^{1/3}64\pi^{2/3}e^2\nu_0^2e^2[2X + 3 - 3(1 + X)^{2/3}]} \right\}^{1/3} \]  \hspace{1cm} (29)

A similar calculation for the slab structure leads to the expressions

\[ E_{SC} = \frac{3}{2} \left( \frac{\pi}{3} \right)^{1/3} \left( \frac{2^{2/3}\pi^{1/3}}{16} \right)^{2/3} K^{2/3} \left( \frac{e^2}{\epsilon_0 a} \right)^{1/3} \nu_0^{4/9} x^{2/3}(1 + x)^{2/9} \]  \hspace{1cm} (30)

\[ L = \left[ \frac{2^{2/3}15(1 + X)^{1/3}\epsilon_0 a}{16\pi^{2/3}e^2\nu_0^2 X^2} \right]^{1/3} \]  \hspace{1cm} (31)

Further calculations should be carried numerically.

Now some results of them will be presented. First, we consider the case when the system is close to the boundary of the polaron instability. For this aim the same values of the dielectric constants will be taken as in EuSe [23]: \( \epsilon_0 = 9.4, \epsilon_\infty = 5 \). As EuSe is an isotropic metamagnet with a very low critical field of about 2000 Oe, a value of \( D = 0.0001 \) is chosen (here and below all the typical energies are in the eV units). Other quantities are: \( t = 0.2, A = 1.2/7, e^2/a = 2.7, S = 7/2 \). Not all they coincide with the corresponding quantities in EuSe though are likely to be close to them. Nevertheless, the inequality \( W \gg AS \) is certainly met here, and the energy of the system will be counted off from the expression (25).

The results of the calculations are depicted in Fig.1 for both droplet and slab structures. Here and below the upper indices \( p \) and \( r \) will denote the polarizable and rigid lattices, the lower indices \( d \) and \( s \) the droplet and slab structures, respectively. The parameters \( X_p^p, X_{d}^d, R^p \) and \( L^p \) are presented in Fig.1 For the droplet model the calculations are carried only down to the \( X^p \) value of 1, which corresponds to the electronic and ferromagnetic percolation. Calculations of the polaronic effects for \( X^p < 1 \) should be carried out using another procedure.

As is seen from Fig. 1, the parameters \( X_d^p \) and \( X_p^p \) decrease and hence the ferromagnetic portion of the crystal increases with increasing charge carrier density \( \nu_0 \). Respectively, the sizes of the ferromagnetic regions \( R^p \) and \( L^p \) increase. For the slab structure an abrupt concentration phase transition
into the uniform ferromagnetic state takes place though the $X^p$ jump is rather small. As the polaronic contribution to the energy is small at $X^p \to 0$, this effect is not related to the polaronic effect. A corresponding calculation for the unpolarized droplet model using results of Refs [3,6] shows that the phase separation also disappears abruptly.

Comparing numerical results for these two models, one should point out that their energies and $X^p$ values are close to each other. In both cases the energy per conduction electron decreases smoothly with increasing electron density. For the droplet structure this energy $E^p_d$ changes from -0.2089 at $\nu_0 = 4 \times 10^{-4}$ ($X^p_d = 5$) to -0.2245 at $\nu_0 = 1.2 \times 10^{-3}$ ($X^p_d = 1$). For the slab structure this energy $E^p_s$ is equal to -0.2058 at $\nu_0 = 4 \times 10^{-4}$ ($X^p_s = 4.6$), -0.2256 at $\nu_0 = 1.2 \times 10^{-3}$ ($X^p_s = 1$), and -0.2387 at $\nu_0 = 1.98 \times 10^{-3}$ ($X^p_s = 0$). It is interesting to note that the densities corresponding to equal volumes of the antiferromagnetic and ferromagnetic phases coincide for both models.

One should compare results obtained with accounting and without accounting for the lattice polarization. It is advisable to carry out this comparison for the density $\nu_0 = 0.00095$ corresponding to the percolation threshold in the rigid lattice. One obtains: for the droplet model in the rigid lattice the energy per electron $E^p_d = -0.2054$, $X^p_d = 1.0$, $R^p_d = 10$, the number of electrons in the droplet $N^p_d = 8.3$. The small parameter of theory ensuring applicability of Eq. (9a) $s^r = 1/[(6\pi^2)^{1/3}\nu_0^{1/3}(1 + x)^{1/3}]$ is 0.21 which justifies use of the many-electron approach adopted here. With accounting for the polaronic effects one has: the energy per electron $E^p_d = -0.2202$, $x^p_d = 1.6$, $R^p = 16$, $N^p_d = 44$, $s^p = 0.12$.

Obviously, the polarization increases the number of the electrons in each droplet by a factor of 4.75, whereas its volume is increased only by a factor of 4.1. Hence, the polarization increases the density of conduction electrons. The total magnetization of the crystal is proportional to the relative volume of the ferromagnetic phase $1/1 + X$. Thus, the polarization decreases the total magnetization by about 30 %. Simultaneously, the system is shifted from the percolation threshold to the insulating side.

Now these results will be compared with those obtained for the slab model with the same $\nu_0$ value of 0.00095. Without polarization, one obtains: $E^s = -0.2073$, $X^s = 1.0$, the ferromagnetic layer thickness $L^f = 8.5$. With polarization, $E^p_s = -0.2208$, $X^p_s = 1.5$, $L^p = 13$. Though, formally, the energy of the slab structure is less than that of the droplet structure, the difference between them amounts only to 0.3 % which is certainly considerably less than
the accuracy of the present calculations. For this reason it is impossible to decide which structure should be realized in reality. The reduction of the magnetization caused by the lattice polarization in the slab structure is close to that in the droplet structure.

Now we consider a double-exchange system of the manganite type with values of the dielectric constants coinciding with those of the La-based manganite: $\epsilon_0 = 5, \epsilon_\infty = 3.4$ [29]. The $s-d$-exchange integral $A$ is assumed to be very large (its exact value is inessential as its enters the expression for the energy only as an additive constant), and the following values will be taken: $t = 0.2, D = 0.01, S = 2$. Then one finds for the density $\nu_0 = 0.015$ close to the percolation density: for the unpolarized droplet structure the energy $E_r^d = -0.06$ is minimal for $X_r^d = 1.1$ with $R_r^d = 4.2, N_r^d = 10$ and $s^r = 0.19$ (the energy is counted off from the energy $U(26)$). If one takes into account the polarization, then $E_p^d = -0.09, R_p^d = 4.8, N_p^d = 16, s^p = 0.17$ with $X_p^d = 1.3$.

In the case of the slab structure for the same values of parameters one finds: for a rigid lattice $E_r^s = -0.0708$ with $X_r^s = 1.1$ and $L_r^s = 3.44$, for a polarizable lattice $E_p^s = -0.0986$ with $X_p^s = 1.3$ and $L_p^s = 3.84$.

As is seen from these data, the main regularities established above for the case of the wide bands $W \gg AS$ remain in force for the case of the double exchange. The difference in the energies of the slab and droplet structures is larger in this double-exchange system case which points to the droplet structure being preferential. One can also give examples where the situation is opposite. Being unable to predict in some cases which structure should be realized, I would like to point out that just due to this small energy difference a small external force can cause transition of one structure to the other. For example, if the droplet structure is normally realized then a small uniaxial stress increasing the hopping integral $t$ in the corresponding direction can stabilize the slab structure.

It is still necessary to discuss the possibility of the ferromagnetic stripe structure ($L = 1$). It is clear that the single layer ferromagnetic phase could be possible only in the double exchange systems since in the opposite case $W \gg AS$ the energy of the two-dimensional motion of the electron is by $2t = W/6$ higher than in the three-dimensional case. Meanwhile, the gain in its energy due to the ferromagnetic ordering is only $AS/2$. On the other hand, as was shown in the preceding section, the polaronic effect is enhanced in the structures with alternating ferro- and antiferromagnetic atomic planes. For this reason one can expect the existence of such structure in the double-exchange systems.
I managed to prove the possibility of such structure in the limit \( S \to \infty \). The following values of the parameters were used: \( \epsilon_0 = 5, \epsilon_\infty = 3.4, t = 0.1, D = 0.01 \). Then one finds from Eqs (6) and (10) that for \( \nu_0 = 0.02 \) the system with \( L^p = 1 \) is the most energetically favored for \( k = 3 \) (3 antiferromagnetic layers per ferromagnetic layer). For \( \nu_0 = 0.05 \) the most energetically favored structure is \( L^p = 1, k = 1 \) with alternating ferro- and antiferromagnetic atomic planes. For small \( S \), I did not find parameter values at which the stripe structure is most energetically favored.

It remains only to consider the magnetostiction deformation of a sample in the case of the slab phase separated state. For this aim one should use Eqs (20), (5b) yielding the shifts \( \beta_q \) of the operators for the longitudinal acoustical phonons. Going over from the phonon operators to the normal coordinates in the standard manner, one obtains the following expression for their shift \( \delta Q_q \):

\[
\delta Q_q = \sqrt{\frac{1}{2\omega_q M}} \left[ \beta_q + \beta^*_q \right]
\]  

(32)

where \( M \) is the mass of the unit cell. Using this Eq, one obtains for the

\[
u_g = A_m \exp(i mg), \quad A_m = \frac{1}{\sqrt{N}}\delta Q_m
\]

As follows from Eq (33), the lattice becomes modulated not only with the

periodicity of the phase-separated structure but also the higher harmonics
are present.

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Captions

Fig. 1. The ratio $X^p$ of the volumes of the antiferromagnetic and ferromagnetic phases for the droplet ($X^p_d$) and slab ($X^p_s$) structures in the polarizable lattice, as well as the radius $R^p$ of the ferromagnetic droplet for the former and the thickness $L^p$ of the ferromagnetic layer for the latter, as functions of the relative average charge carrier density $\nu_0$. $R^p$ and $L^p$ are expressed in the lattice constants. Numerical values of the parameters used, which correspond to $W \gg AS$, are presented in the text just below Eq. (31).