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SOLID STATE PHYSICS

NONEQUILIBRIUM MICROSCOPIC TREATMENT OF THE ORDERING PROCESS
IN A SOLID SOLUTION

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and V. E. Panin

A phase transition of the type "order—disorder" has been considered in solid solutions within the framework of the electronic subsystem as a collection of quasiparticles called "concentrons" in a state with a wave vector which is equal to the wave vector k_S of the superstructure; the phase transition is due to emission of concentrons when relaxation of electronic bands of atoms on "foreign" sublattices takes place. This treatment permitted a simple description of the ordering kinetics on a microscopic level. In this work, the possibility of creation of dissipating structures in solid solutions is also discussed. Conditions for the occurrence of these structures have been analyzed. The mechanism of formation of a structure of A_2B type has been explained for the case of tempering of binary solid solutions which have a tendency to order into the CsCl structure.

INTRODUCTION

Recently, the method of concentration waves [1] has been widely used in the study of ordering processes of solid solutions. This method allows one to determine the structure of the ordered state and to calculate thermodynamic characteristics for arbitrary values of the long-range order parameter. An alternative approach to the study of the phase transition is based on the concept of quasiparticles in an atomic system [2]. In terms of these quasiparticles, a "disorder—order" phase transition is represented as their Bose-condensation in a state with a wave vector, which is equal to the superstructure wave vector k_S. Neither of these methods considers microscopic properties and reasons for ordering, which are ultimately determined by the electronic subsystem. There have been attempts for a quantum description of ordered solid solutions which allow one to perform a calculation of a number of energy parameters within the framework of the pseudopotential method and to determine superstructure vectors which are determined by the geometry of the Fermi surface. In this case, the reason for ordering is also related to the features of the Fermi surface [3].

A study of the electron spectrum of a binary ordering alloy, performed in [4, 5], has shown that the ordering (disordering) process is due to the character of the behavior of atomic bands on "foreign" sublattices ("impurity" bands). Figure 2 of [4] shows the electron spectrum of FeCo solid solution for various values of the long-range order parameter η; the dashed region indicates the "impurity" band. These bands can be considered as an excited state of the electron subsystem, maintained by the temperature of the thermostat. As temperature is lowered, the number of electrons occupying such an excited state decreases, i.e., they return to their "own" bands by emitting concentrons with $k = k_S$. Consequently, the ordering process of a solid solution can be considered, within the framework of the electron subsystem, as accumulation of concentrons in k_S-condensate due to their emission during relaxation of excited electron states ("impurity" bands), and the disordering process can be considered as an excitation of the electron subsystem after absorbing concentrons with $k = k_S$.

1. ELECTRON—CONCENTRON INTERACTION HAMILTONIAN

In order to describe the phase transition, we shall write down the Hamiltonian for the interaction of electrons with the crystalline field of an ordering binary alloy as follows:

$$H_{e-i} = \sum_{R,R',s} V_s(R - R')\, \Psi^+(R)\, \Psi(R)\, C_s(R'), \tag{1}$$

where s is the atom kind; $V_s(r)$, lattice site potential; $\Psi^+(R)$, $\Psi(R)$, electron field operators; $C_s(R)$, microscopic concentration of atoms of s-th kind ($C_a(\mathbf{R}) + C_b(\mathbf{R}) = 1$).

For simplicity, we shall consider a binary alloy and shall assume that the ordering process is characterized by a single-order parameter η: In the disordered state, the crystalline lattice is a simple one, and in the ordered state it is a cell with a basis R and sites p = 1, 2.

Let us modify Eq. (1) so that the electron—concentron interaction can be clearly distinguished. Introducing the function δC(R) = C(R) — C (C is the macroscopic concentration), which describes redistribution of atoms, Eq. (1) can be rewritten as follows:

$$H_{e-i} = \sum_{R,R'} [V_a(R - R') + Cg(R - R')]\, \Psi^+(R)\, \Psi(R) + \sum_{R,R'} g(R - R')\, \Psi^+(R)\, \Psi(R)\, \delta C(R'); \tag{2}$$

$$g(R - R') = V_a(R - R') - V_b(R - R').$$

The first term in Eq. (2) has a diagonal form and causes only renormalization of the electron energy. The second term describes the electron—concentron interaction. Indeed, operator δC(R) can be expressed through concentron field operators $\varphi^+(R)$ and $\varphi(R)$ [2]; in this case one obtains

$$H_{e-e} = \frac{\sqrt{C(1-C)}}{2} \sum_{R,R'} g(R - R')\, \Psi^+(R)\, \Psi(R)\, [\varphi^+(R') + \varphi(R')]. \tag{3}$$

Let us rewrite Eq. (3) in k-representation by introducing concentron creation and annihilation operators b^+_q and b_q in state q:

$$H_{e-e} = \sum_{\kappa,q} \Delta(q)\, (a^+_{\kappa+q} a_\kappa b_q + a^+_\kappa a_{\kappa+q} b^+_q), \tag{4}$$

where

$$\Delta(q) = \sqrt{C(1-C)}\, g(q)/2\sqrt{N},$$

a^+_k, a_k are electron creation and annihilation operators. We note that operators b^+_k and b_k are quasi-Bose operators [2] so that

$$b_\kappa b^+_{\kappa'} - b^+_{\kappa'} b_\kappa = \delta_{\kappa,\kappa'}(1 - 2C + \eta^2/2) - \frac{\eta^2}{2}\delta_{\kappa-\kappa',\kappa_s}. \tag{5}$$

Since we are interested in the interaction of electrons with concentrons in state k_s, henceforth we shall use the following Hamiltonian:

$$H_{e-e} = \sum_\kappa \Delta(\kappa_s)\, (a^+_{\kappa+\kappa_s} a_\kappa b_{\kappa_s} + a^+_\kappa a_{\kappa+\kappa_s} b^+_{\kappa_s}). \tag{6}$$

It is easy to see that in the equilibrium state interaction (6) in an ordering system leads to appearance of a gap in the electron spectrum [4]. On the other hand, as will be shown in the present work, under nonequilibrium conditions Eq. (6) determines generation of electrons with $k = k_s$.

Let us now write down the full Hamiltonian of the electron—concentron system:

$$H = \sum_\kappa \varepsilon_\kappa a^+_\kappa a_\kappa + \left\{ \left[\frac{1}{4} C(1-C) w(\kappa_s) - \mu \right] b^+_{\kappa_s} b_{\kappa_s} + \right.$$

$$\left. + \frac{1}{8} C(1-C) w(\kappa_s) (b^+_{\kappa_s} b^+_{-\kappa_s} + b_{\kappa_s} b_{-\kappa_s}) \right\} + \sum_\kappa \Delta(\kappa_s)\, (a^+_{\kappa+\kappa_s} a_\kappa b_{\kappa_s} + a^+_\kappa a_{\kappa+\kappa_s} b^+_{\kappa_s}). \tag{7}$$

The expression in curly brackets of Eq. (7) is the Hamiltonian for free concentrons [2]; μ is the concentron chemical potential; $w(k_s)$ is the Fourier image of the mixing energy.

2. KINETICS OF ORDERING OF A SOLID SOLUTION

The ordering process of a solid solution can be described in the following way: As temperature is lowered from T_c (Kurnakov temperature) to some temperature T_1, electrons from the "impurity" band start returning to their "own" bands, accompanied by emission of concentrons with $k = k_s$. This leads to the appearance of the concentron condensate with $k = k_s$ (k_s refers to the condensate), i.e., there appears initially a nonequilibrium long-range order parameter η, and the number of electron states in the "impurity" band is further reduced.

The latter process will take place until the system reaches the state having the equilibrium long-range order parameter at the given temperature T_1. In order to find the time dependence of the long-range order, and, consequently, the equilibrium value of η, it is sufficient to consider relaxation of the system in which at the initial moment in time there is a nonzero difference of the number of states σ^o_{k,k_s} created with k and $k = k_s$. Let us write down the Heisenberg equation of motion for concentron operators $b^+_{k_s}$ and b_{k_s}, electron polarization $d^+_{k,k_s} = a^+_{k+k_s}a_k$ and $d_{k,k_s} = a^+_k a_{k+k_s}$, and for the occupation difference $\sigma_{k,k_s} = a^+_{k+k_s}a_{k+k_s} - a^+_k a_k$:

$$\dot{b}^+_{\kappa_s} = i\left[\frac{1}{4}C(1-C)w(\kappa_s) - \mu\right]\alpha b^+_{\kappa_s} + i\Delta(\kappa_s)\alpha\sum_\kappa d^+_{\kappa,\kappa_s};$$

$$\dot{d}^+_{\kappa,\kappa_s} = (i\omega_{\kappa,\kappa_s} - \Gamma_{\kappa_s})d^+_{\kappa,\kappa_s} - i\Delta(\kappa_s)b^+_{\kappa_s}\sigma^0_{\kappa,\kappa_s}; \quad (8)$$

$$\dot{\sigma}_{\kappa,\kappa_s} = -\sigma_{\kappa,\kappa_s}t_\sigma^{-1} + 2i\Delta(\kappa_s)(b^+_{\kappa_s}d_{\kappa,\kappa_s} - b_{\kappa_s}d^+_{\kappa,\kappa_s}).$$

In this case, $\dot{b}_{k_s} = (\dot{b}^+_{k_s})^+$, $\dot{d}_{k,k_s} = (\dot{d}^+_{k,k_s})^+$, $\omega_{k,k_s} = \varepsilon_{k+k_s} - \varepsilon_k$, $\alpha = (1 - 2C + \eta^2/2)$ is a factor due to the quasi-Bose character of operators $b^+_{k_s}$ and b_{k_s}.

In Eqs. (8) we neglected terms proportional to $b^+_{-k_s}$ and b_{-k_s} because below we will be interested in average values, and $<b^+_{-k_s}> = 0$ and $<b_{-k_s}> = 0$. Dissipation processes in Eq. (8) have been taken into account phenomenologically, and for this reason dumping of pairs of electron states Γ_{k,k_s} and the relaxation time t_σ of the electron occupation numbers have been introduced; transitions between electron states within pairs take place by emitting a concentron with $k = k_s$. We neglected dumping of concentrons with $k = k_s$ because concentrons that are in condensate are practically not dumped.

Let us average Eqs. (8) with the help of the density matrix. Since the number of emitted concentrons will be macroscopic, for averaging Eqs. (8) it is sufficient to replace operators by their average values [6]. Below, it is assumed that such a replacement has been performed and the notation has been left the same. In order to get rid of the oscillating time dependence, one should introduce new variables:

$$\tilde{b}^+_{\kappa_s} = e^{-i\omega_{\kappa_s}t}b^+_{\kappa_s}; \quad \tilde{b}_{\kappa_s} = e^{i\omega_{\kappa_s}t}b_{\kappa_s};$$

$$\tilde{d}^+_{\kappa,\kappa_s} = e^{-i\omega_{\kappa_s}t}d^+_{\kappa_s}; \quad \tilde{d}_{\kappa,\kappa_s} = e^{i\omega_{\kappa_s}t}b^+_{\kappa_s}, \quad (9)$$

In this case we shall consider the case of the exact resonance

$$\omega_{\kappa_s} = \omega_{\kappa,\kappa_s} = \left[\frac{1}{4}C(1-C)w(\kappa_s) - \mu\right].$$

Upon substituting Eq. (9) into Eq. (8) the latter takes the form

$$\dot{\tilde{b}}^+_{\kappa_s} = i\Delta(\kappa_s)\alpha\sum_\kappa d^+_{\kappa,\kappa_s};$$

$$\dot{\tilde{d}}^+_{\kappa,\kappa_s} = -\Gamma_{\kappa_s}\tilde{d}^+_{\kappa,\kappa_s} - i\Delta(\kappa_s)\tilde{b}^+_{\kappa_s}\sigma_{\kappa,\kappa_s}; \quad (10)$$

$$\dot{\sigma}_{\kappa,\kappa_s} = -\sigma_{\kappa,\kappa_s}t_\sigma^{-1} + 2i\Delta(\kappa_s)(\tilde{d}_{\kappa,\kappa_s}\tilde{b}^+_{\kappa_s} - \tilde{d}^+_{\kappa,\kappa_s}\tilde{b}_{\kappa_s})$$

and $b^+_{k_s} \approx \tilde{b}_{k_s} \approx \sqrt{N_s}$, with $\eta = \sqrt{N_s/N}$, where N_s is the number of concentrons in condensate and N is the total number of concentrons.

Initial conditions for system (10) are

$$\tilde{b}^+_{\kappa_s}\big|_{t=0} = \tilde{b}_{\kappa_s}\big|_{t=0} = 0; \quad \sigma_{\kappa,\kappa_s}\big|_{t=0} = \sigma^0_{\kappa,\kappa_s}; \quad d^+_{\kappa,\kappa_s}\big|_{t=0} = d^+_0,$$

where d^+_0 is the average value of the polarization operator at the initial moment in time.

The system of equations is a nonlinear one and can be solved only numerically, with the corresponding choice of the macroscopic parameter. Analysis of equations shows increase in the order parameter is caused by the electron-concentron interaction. The rate of change of η with time decreases, on one hand, due to the fact that at $t \to \infty$ d^+_{k,k_s} is equal to zero, and increases, on the other hand, due to increasing Δ and α as η increases. The difference of occupation numbers, σ_{k,k_s}, will decrease as η increases, due to concentron emission.

In solving Eq. (10) numerically, one should take into account the dependence $\Delta(\eta)$, which can be obtained by analogy with [4]. From the solution of Eq. (10), one can obtain the connection between σ^0_{k,k_s} and the equilibrium value of the long-range order parameter by calculating the limit of $\eta(t)$ as $t \to \infty$.

Thus, treatment of the ordering process of a solid solution as relaxation of the "impurity" band allows one to describe in a rather simple way kinetics of ordering on a microscopic level.

3. STATIONARY DISSIPATIVE STRUCTURES IN SOLID SOLUTIONS

The proposed approach to the treatment of ordering processes allows one to predict also the existence of dissipative structures which exist only under nonequilibrium conditions.

Under nonequilibrium conditions such as in the presence of a temperature gradient, there appear inversely populated electron states. As a result of this, electron transitions become possible accompanied by a change of the inverse population. Some of these transitions will take place accompanied by concentron emissions; in this case, the number of transitions taking place along the concentron channel will be greater the greater $\Delta(q)$ is. If the number of pairs of inversely populated states, which have the same difference between wave vectors $k'-k = q$, is macroscopic, then there could appear, as a result of generation, a concentron condensate with wave vector equal to q, which means that ordering with respect to the star $q = k' - k$ is possible. Such nonequilibrium states can appear only from an ordered equilibrium state considered earlier. This is due to the fact that in a nonequilibrium state transition along the concentron channel cannot take place because $\Delta(q)$ is equal to zero. Appearance of the q-condensate will be precluded by dumping of $\varkappa_q$ of concentrons; however, for a large inverse population in a solid solution, there could exist two concentron condensates with $k = k_s$ and $k = q$. In general, due to concentron generation by the nonequilibrium electron subsystem, there could appear several condensates with $k = q, q', \ldots$, i.e., complex dissipative superstructures will be formed.

Let us construct a microscopic description of the appearance of the condensate. For simplicity we shall restrict ourselves to the treatment of only one condensate with $k = q$, i.e., we shall consider the interaction of electrons only with q-concentrons, and shall not consider interaction of q- and k_s-condensates. Let there exist in a partially ordered solid solution with an equilibrium (infinitesimally small) value of the order parameter nonequilibrium conditions such as a temperature gradient. Let us maintain the nonequilibrium state for a certain duration. This can be done by placing the system between two thermostats having temperatures T_1, $T_2 < T_c$.

Under these conditions, there appears in the system inverse population $\sigma^0_{k,q}$ of electron states which does not depend on time; it is greater when $|T_1 - T_2|$ is greater. In order to describe the appearance of a dissipative structure, we will write down, as we did earlier, the Heisenberg equations of motion for operators b^+_q, b_q, $d^+_{k,q}$, $d_{k,q}$, $\sigma_{k,q}$. Unlike Eq. (10), in the present equations it is necessary to include the inverse population $\sigma^0_{k,q}$ and the concentron dumping $\varkappa_q$. After transformations, analogous to those performed in deriving Eq. (10), we have:

$$\varkappa_q \tilde{b}^+_q - i\Delta(q)\alpha \sum_\varkappa \tilde{d}^+_{\varkappa,q} = 0;$$

$$\varkappa_q \tilde{b}_q + i\Delta(q)\alpha \sum_\varkappa \tilde{d}_{\varkappa,q} = 0;$$

$$\Gamma_q \tilde{d}^+_{\varkappa,q} + i\Delta(q) \tilde{b}^+_q \sigma_{\varkappa,q} = 0; \tag{11}$$

$$\Gamma_q \tilde{d}_{\varkappa,q} - i\Delta(q) \tilde{b}_q \sigma_{\varkappa,q} = 0;$$

$$(\sigma^0_{\varkappa,q} - \sigma_{\varkappa,q}) t^{-1}_\sigma + 2i\Delta(q)(\tilde{b}^+_q \tilde{d}_{\varkappa,q} - \tilde{b}_q \tilde{d}^+_{\varkappa,q}) = 0.$$

The stationary solution $\sigma_{k,q}$ corresponds to the case when increases and losses compensate each other, and therefore, it plays the role of the threshold difference between populations $\sigma^{th}_{k,q}$. From the condition for the existence of a nonvanishing solution for $\tilde{b}^+_q$ and $\tilde{b}_q$ we find:

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$$\sum_{\varkappa} \sigma_{\varkappa,q}^{th} = \frac{\varkappa_q \Gamma_\sigma}{\Delta^2(q)\,\alpha}\ .$$

In the presence of a macroscopic number of inversely populated pairs of states with $k' - k = q$ one can write down

$$\sigma_q^{th} \simeq \frac{\Gamma_q \varkappa_q}{n_q \Delta^2(q)\,\alpha}, \tag{12}$$

where σ^{th}_q is the threshold difference between populations within a pair of states, the transition between which takes place with emission of a concentron with a wave vector q; n_q is the number of such pairs of states. It is seen from Eq. (12) that the threshold will be smaller when Γ_q^{-1}, $\varkappa_q^{-1}$, $\Delta(q)$, α, as well as the number of inversely populated pairs n_q, are larger. Using the last three equations in system (11), and taking into account that $b^+_q b_q = N_q$, we will obtain the following expression:

$$N_q = \frac{\Gamma_q}{4 t_\sigma \Delta^2(q)} \left(\frac{\sigma_q^0}{\sigma_q^{th}} - 1 \right). \tag{13}$$

For $\sigma^0_q < \sigma^{th}_q$, there is no stationary state containing the condensate, and for $\sigma^0_q > \sigma^{th}_q$, there will be a condensate containing N_q concentrons, i.e., the long-range order parameter $\eta_q = \sqrt{N_q/N}$ and N_q will be macroscopic because $\Delta^2(q) \sim N^{-1}$. In order to analyze the dependence of η_q on parameters, determining the electron–concentron system, we shall rewrite expression (13) in the following form:

$$\eta_q^2 = \frac{\sigma_q^0 n_q (1 - 2C + \eta^2/2)}{4 t_\sigma \varkappa_q N} - \frac{\Gamma_q}{C(1-C)\,g^I(q) t_\sigma}. \tag{14}$$

It is seen from Eq. (14) that, in the general case, η_q depends on η in a nonlinear fashion. If t_σ^{-1} and $\varkappa_q$ are of the same order of magnitude, then for $\sigma^0_q \gg \sigma^{th}_q$ the following expression is valid:

$$\eta_q^2 \sim \frac{\sigma_q^0 n_q}{N} (1 - 2C + \eta^2/2).$$

Consequently, for the existence of dissipative structures, it is necessary to have the following: macroscopic n_q and a high inverse population σ^0_q.

Dissipative structures of this type can be formed during tempering of solid solutions. If tempering is done by cooling to sufficiently low temperatures, then dissipative structures that appear could "freeze" and continue to exist in the absence of external nonequilibrium conditions. This is possible because of the fact that, although these "frozen" states are nonequilibrium states, their relaxation time at low temperatures will be very long.

An example of dissipative structures, whose formation was considered in the present paragraph, is, apparently, a structure of the type A_2B (the star $Q = 2\pi/3a\,(121)$), which is formed during tempering of solid solutions which have a tendency towards ordering into a structure of CsCl type (e.g., see [7]). This fact, obviously, has a direct relation with the fact that for $\eta \neq 0$, in the electron spectrum of these solid solutions, in addition to superstructure gaps at the point $k_s = 2\pi/a\,(111)$, there opens a gap at the point $Q = 2\pi/3a\,(121)$ (see Fig. 2b of [4]). The existence of this gap and formation of structures of A_2B type can be explained on the basis of the same principles, with the help of ideas developed in the present work.

The symmetry of the ordered crystal CsCl is such that there exist in the electron subsystem a macroscopic number of pairs of electron states which have wave vectors $k + Q$ and k, and transitions between these states are allowed within the concentron channel. In the equilibrium state, transitions between these states will create a virtual condensate consisting of concentrons with $k = Q$. Interaction of electrons with this condensate will lead to the appearance of a gap at the point Q. This treatment of the gap formation can be performed analogously to Sec. 7 of [4]. Since for $\eta = 0$ $\Delta(Q) = 0$, this gap does not appear in a nonequilibrium state because of the absence of transitions taking place within the concentron channel. Due to the fact that the concentron condensate with $k = Q$ is virtual, the structure with the star $2\pi/3a\,(121)$ will not be observed in an equilibrium state.

The situation becomes quite different if nonequilibrium conditions are created in the system (this take place during tempering). Under nonequilibrium conditions there appears inverse population between states with wave vectors $k + Q$ and k. As a result of this, the system will begin to generate concentrons with $k = Q$, and this will lead to the appearance

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of Q-condensate, i.e., a structure of A_2B type will appear which can be "frozen" upon further cooling to $T \ll T_C$.

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GRAIN-BOUNDARY HARDENING IN POLYCRYSTALLINE COPPER-BASED

SOLID SOLUTIONS

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A study is made of the contribution of grain-boundary hardening to the overall hardening in a polycrystalline material on the basis of Ashby's model. Yield curves are used for copper-based solid solutions in polycrystalline and single-crystal forms. It is shown that the contribution from statistically accumulated dislocations to the yield stress in a polycrystalline specimen reflects the behavior of the corresponding single crystal. The contribution from grain boundaries to the yield stress can be described in terms of the additional dislocation density due to the joint grain deformation in the aggregate up to high strains. At low strains, the main role in hardening of a polycrystalline material is played by the grain boundaries. This extends up to larger strains as the strain temperature is reduced and the alloy-element concentration increases.

In the analysis of polycrystalline-material plastic-strain mechanisms, it is important to estimate the role of grain-boundary hardening in the overall yield stress level. There are two approaches to estimating the contribution from the grain boundaries to the hardening. Firstly, there is the empirical Hall—Patch relationship [1]

$$\sigma = \sigma_\infty + Kd^{-1/2}, \tag{1}$$

which has been given a theoretical basis in various studies dealing with the stress concentration at the head of a planar dislocation group. In that case, the grain-boundary hardening is distinguished from the general level of yield stress in the polycrystalline material. However, there are no planar dislocation groups at medium and high strains [2], so the planar-group model as a fundamental yield mechanism is doubtful.

The other approach is based on the established experimental fact that the yield stress is

$$\sigma = \sigma_0 + \alpha G b m \rho^{1/2}, \tag{2}$$

where σ_0 is a frictional stress of nondislocation character; ρ, average dislocation density; and α, G, b, and m, constants.

In that case, the yield stress is related not directly to the grain size but via the dislocation density. The dependence of the yield stress on grain size was incorporated