

LONG-PERIOD STATES OF ORDERED INTERMETALLIC ALLOYS.

2. PHYSICAL REPRESENTATION OF THE NATURE OF THEIR FORMATION

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A survey of the empirical data shows that there are two fundamentally different groups of long-period alloys. An analysis of the physical representations leads to the conclusion that their long-period states are different in nature. The stabilization of this state is determined by relaxation processes in one group and by competing interactions in different coordination spheres in the other group.

A substantial amount of empirical data has now been accumulated on the structure and behavior of long-period states (LPSs), which were analyzed in detail in the first part of this article [Izv. Vyssh. Uchebn. Zaved., Fiz., No. 6, 3-21 (1995)]. It follows from the analysis that the class of LPSs is actually comprised of two groups of alloys differing in structural features and behavior.

The following can be considered the most important features of alloys of the first group (CuAuII, Cu_3AuII , Au_3CuII , one- and two-dimensional LPSs in Cu_3Pd and their analogs) from our viewpoint:

- the ordered low-temperature phase is realized in the form of a base superstructure (such as $L1_2$, $L1_0$, etc.);
- relaxation effects (local changes in composition, variation of the degree of long-range order, lattice modulation) are seen in the neighborhood of the periodic antiphase boundaries (APBs), i.e., the APBs are spread out over 2-3 atomic planes;
- the LPS is manifest as a disproportionate equilibrium structure in a temperature range near the order–disorder transition (T_c). The size of the half-period is generally greater than 5 unit cells of the base superstructure.
- external conditions (composition, pressure, alloying, temperature) have a significant effect; variation of these conditions is accompanied by a continuous change in the mean size of the antiphase domains (the LPS half-period) M . It decreases with an increase in temperature up to T_c and a change in composition up to the equiatomic composition.

The following features are intrinsic to the second group of alloys (Ag_3Mg , Au_3Mn , Al_3Ti , Pt_3V , and their analogs):

- the low-temperature phase is realized in the form of a proportionate long-period structure relative to the base superstructure (for example, $D0_{22}$ or $D0_{23}$ relative to $L1_2$);
- the high-temperature state is formed as a regular set (if "disproportionate" LPSs are formed) of proportionate structures that are readily resolved in the patterns seen in structural studies. The one-domain structure often remains present up to T_c ;
- the "mean size" of the antiphase domain is characterized by rational numbers with a change in the composition of the alloy and temperature. It tends to increase with temperature. Mean size generally does not exceed 2.5 in the disproportionate state;
- no significant relaxation effects are usually seen in the neighborhood of periodic APBs. A slight displacement of atoms from the lattice points is seen in isolated cases.

The analysis performed in the first part of this investigation gives every reason to conclude that the first and second long-period states are fundamentally different in character. In this part of the study, we will analyze physical representations of the nature of the formation and behavior of LPSs.

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PHYSICAL REPRESENTATIONS OF THE NATURE OF LPSs

No single physical representation has as yet been agreed upon as regards the nature of the stability of ordered alloys with a long period. As a result, there are several approaches to explaining the formation of LPSs. We will examine some of them here, giving special attention to the most recent research.

It is generally accepted that the formation of LPSs is connected with ordering. Most of the studies that have examined different aspects of the ordering process have been conducted using the traditional model [1-5], which is based on the following approximations:

- the atomic lattice of the alloy is assumed to be rigid, i.e., it does not undergo local distortions in the transition from one structural state to another;
- the interaction of atoms in the lattice is assumed to be paired and central, and it does not change during phase transformations;
- it is assumed that the interaction of nearest neighbors is important, and limited allowance is made for this factor.

Of decisive importance in the model is the formation, based on the given lattice and with the given alloy composition, of a superstructure in which the largest number of pairs of different types of atoms, i.e., A–B pairs, is formed as a result of an order–disorder transformation.

Since unidimensional LPSs with the base superstructure $L1_2$ have only APBs whose formation does not result in changes in the nearest-neighbor atoms, the formation of LPSs cannot be explained within the framework of the traditional theory of ordering. Changes begin with the next nearest-neighbor, so it was assumed earlier that the energy of interaction of next nearest-neighbor atoms plays the main role in the stabilization of LPSs [2, 7, 8]. Efforts made to expand the traditional model and attribute nearest-neighbor ordering to additional ordering in the second neighborhood failed to yield an equilibrium ordered phase with periodic APBs [9].

Studies conducted within the framework of the thermodynamic phenomenological model do not require knowledge of the thermodynamic potential (model) and are based solely on symmetry considerations. This theory was used in [10, 11] to examine long-period phases that are formed and disappear in second-order transitions. The nonequilibrium potential accounts only for that part determined by generalized elastic moduli. It was found in [10] that an LPS should have several properties within the range of values in which the given approach is valid: the transition from a highly symmetric structure in the LPS should be a second-order transition; the long period should depend appreciably on temperature; the LPS is located near the boundary of stability of the phase with the base superstructure, in which there are few structural distortions.

The application of the Landau theory to CuAu alloys with an LPS [12] predicts that the transition from the disordered state to the LPS will be a second-order transition. This contradicts the available experimental data [7], which indicates that the transition from an LPS to a state with the base superstructure will be a first-order transition. In this case, there is a very slight change in the long period in the region of the LPS.

The cycle of studies [13-16] was conducted within the framework of a semi-phenomenological model of distorted solid solutions. Force constants were used as parameters, and these constants contain contributions from interatomic interaction and the electron energy of the alloy. Free energy was expanded into a series in static displacements in a harmonic approximation.

The longwave method was used in [16] to obtain general expressions for uniform and nonuniform elastic strains occurring during the ordering of substitutional alloys. The model gives results close to the experimental findings for uniform strains due to the formation of an LPS. At the same time, the model cannot usually even predict the direction of the mean static displacements.

Steady states in inhomogeneous ordered binary alloys were studied in [17] on the basis of Euler's nonlinear equation. The periodic solution to this equation can be identified as representing long-period superstructures with a nonintegral modulation period.

All of the phenomenological approaches require little information on the system in which the LPS is formed, but they do not shed much light on the physical reasons for the formation of ordered long-period structures.

A promising direction of research into the nature of LPSs in alloys lies in approaches that connect the formation of an LPS with features of the electronic structure of the ordered alloy.

An analysis of the type of theory that might be able to explain the formation of LPSs [18] showed that the theory should be an equilibrium theory and should account for the collective behavior of the crystal in some form. This means that the theory should describe the collective behavior of free (valence) electrons or certain cooperative behavior by the atoms [18].

Experiments have established a link between the electron concentration of an alloy and the long period of the LPS. It was suggested on this basis that collective behavior by valence electrons is responsible for the formation of structural states with equilibrium APBs. It was proposed in [19] that free electrons play a role in stabilizing phases in alloys, and it was suggested that the energy of the electron subsystem decreases when the Fermi surface touches the boundary of a Brillouin zone. This proposition was explored further in [20], where it was proposed that an increase in the translation period during ordering leads to division of the original Brillouin zone into smaller zones. The sizes of the new Brillouin zones are determined by the new translation period. The division of the original zone stabilizes the superstructure, the period of the superstructure being such that the boundaries of the new zones touch the boundary of the Fermi surface. There is an accompanying reduction in the energy of the valence electrons of the alloy. This mechanism of stabilization of new superstructures has been used in studies of alloys with a large unit cell. The successes achieved as a result have stimulated researchers [7, 18, 21, 22] to attempt to use the same approach to explain the stabilization of structures with quasi-periodic APBs.

These approaches are based on the assumption that new gaps appear in the energy spectrum of the valence electrons. The energy of the entire system is reduced as a result of the interaction of the Fermi surface with the planes of new Brillouin zones. The electron redistribution that takes place in this case leads to the appearance of new peaks on the density-of-states curve and tends to stabilize a structure with equilibrium APBs [23-26].

The authors of [9, 18] presented results from empirical substantiation of the physical patterns seen in the formation of LPS. It was noted that the form of the Fermi surface can vary quite broadly. For example, nearly plane sections are formed in the $\langle 110 \rangle$ direction in the alloy Cu_3Au [9]. An attempt to construct an electronic theory of the stabilization of long-period structures [25], done using CuAuII as an example, confirmed the important role of plane sections on the Fermi surface within the framework of the given theory. It was shown that the energy of the ordering that occurs due to interactions between ions makes the structures of CuAuI and CuAuII more stable compared to other superstructures, although no energy differences have been observed between these superstructures. Similar calculations were performed later for alloys of the systems Cu-Pd and Cu-Pt near the composition A_3B , in which unidimensional and two-dimensional LPSs are formed [26, 27]. These studies considered three components of the energy of an alloy: the repulsive energy between nearest neighbors; the ordering energy, following from the behavior of the valence electrons; the elastic energy associated with lattice distortion. It was found that the first two components help stabilize a structure with a long period. Later investigations conducted with allowance for the actual Fermi surface [28-39] showed that groups of collectivized electrons localized near sections of the Fermi surface with small radii of curvature must be responsible for the formation of a structure with equilibrium APBs.

Serious complications arise in the given approaches when an attempt is made to explain the equilibrium of the state of alloys with an LPS. Several calculations performed for the alloys Cu_3Au and Au_3Cu showed [40] that the energy of the LPS is greater than the energy of the base superstructure L1_2 . It was concluded from this that, due to the entropy factor, an LPS should be higher with respect to temperature on the constitution diagram than L1_2 . This conclusion does not seem very convincing in light of studies of the nature of the formation of LPSs. At the very least, the next argument [41, 42] raises additional doubts. It was established experimentally that, with a decrease in temperature, LPSs of the first type are always formed directly from the disordered phase, without passing through intermediate structural states of the type L1_2 or L1_0 . Thus, the thermodynamic potential and the heat of formation of an ordered phase with the superstructure L1_2 or L1_0 are lower than the corresponding characteristics of a phase with an LPS. This conclusion – which follows from experimental data – is in conflict with the theory examined above. The latter holds that the enthalpy of a short-period phase will be greater than the enthalpy of a phase with an LPS due to a reduction in the energy of the LPS resulting from a decrease in the kinetic energy of the conduction electrons. Thus, it is necessary to include some kind of energy term when studying the stability of LPSs of the first type. A similar conflict with this theory was noted in [43] for CuAu alloys of nonstoichiometric composition, as well as for Ag alloys in which the electron/atom ratio does not change with composition and concentration effects play an important role in the stabilization of periodic APBs.

The investigation [44] is of particular interest in this regard. Here, mean-field theory was used to study nonstoichiometric Cu-Au alloys near the composition CuAu . The following contributions to the free energy of the system were taken into account: conduction electrons, the repulsive interaction of atom shells, lattice distortion, and entropy. All of these contributions depend on concentration modulation. It was found that phase transformations of the " CuAuI-CuAuII – disordered phase" type are first-order transitions, which is consistent with the experimental data. Long-period structures with a uniform distribution of excess atoms have proven to be unstable against modulation of composition in the long-period direction. The magnitude of the concentration modulation period is the half-period of the LPS, and excess atoms tend to migrate

to the APB. It must be emphasized that concentration modulation plays an important role in stabilizing LPSs: it either helps stabilize LPSs or is responsible for their very formation.

The approach used in [45] is promising for examining the nature of alloys with an LPS. Here, the formation of disproportionate states is linked with displacements of atoms from their ideal positions in the lattice.

Another well-known hypothesis used as a basis for attempts to explain the formation of structures with equilibrium APBs entails the construction of a model containing the following basic assumptions [46-50]: the valence electrons of the alloy form a certain electron lattice similar to the atomic lattice; the formation of the electron lattice leads to a reduction in the energy of the electron gas; the atomic and electron lattices are governed by strict relations, and any deviation from these relations results in distortion of one of the lattices. The electron sublattice is of primary importance, and changes in it leads to distortions (shear distortions, for example) of the atomic lattice of the alloy. The model assumes the existence of a highly correlated system of free electrons. As in the ionic-bond model [46], this results in the formation of certain electrostatic fields. A singular three-dimensional localization of each valence electron is introduced in place of the nearly uniform distribution of free electrons examined in metals and alloys. A deviation from strict correspondence between the electron and atomic lattices occurs when there is a deficit or excess of valence electrons. In accordance with the given model, this situation in turn leads to the formation of a new translation period in the atomic lattice. The establishment of the new period restores the exact correspondence between the atomic and electron lattices, and a structure with equilibrium APBs is formed in the alloy. A large amount of experimental data [46] on structures with a long period was reviewed to support this conclusion. The analysis revealed an approximately linear relationship between the density of shears (the density of APBs) and the density of valence electrons, as should be expected from the model. However, since these are purely empirical representations, the linear relationship cannot be considered direct proof of the postulates of the model [7]. Moreover, additional assumptions must be made in order to explain other characteristics of LPSs.

Let us examine one more direction being taken in the construction of models that link the formation of LPSs with the excess of entropy in a long-period structure compared to the normal structure [7]. One possible explanation for the excess entropy was given in [51], where it was suggested that entropy contributes to the formation of thresholds for APBs [52]. It was shown later [53] that this notion cannot explain the entropy excess and, thus, the formation of LPSs at high temperatures. It was concluded in [53, 54] that the excess entropy in LPSs cannot be attributed to the excess entropy of APBs on the basis of the model of nearest-neighbor interaction. A subsequent analysis made using cluster variation method [55] showed that the stability of LPSs at finite temperatures cannot be ascribed simply to the entropy inside a single antiphase boundary in an approximation that includes only the interaction of nearest neighbors. A similar conclusion was reached in [56, 57] in the use of the Monte Carlo method and Ising's antiferromagnetic model for the nearest neighbors in an fcc lattice.

We should also mention the microscopic models constructed to explain the nonintegral values of the mean half-period of LPSs, i.e., \bar{M} . Two directions can be discerned in this research. In the Fujiwara model [58], describing a "regular distribution with a uniform mixture," the half-periods M have only rational values and it is assumed that all of the APBs are of planar form. In the other model [59], the orthogonal wave function is replaced by a smooth "order function" with the period $2M$. This function gives the probability of the replacement of one of the sublattices by a certain element in the planes perpendicular to the modulation direction (Jehanno model). The APBs become wavelike in character in this model. Refinements of each model [60-62] were discussed in [42, 63, 64] with reference to Ag_3Mg and CuAuII . It was concluded that the Fujiwara model is more appropriate for Ag_3Mg , i.e., alloys with LPSs of the second type, and that the Jehanno model more closely describes alloys of the type CuAuII , i.e., alloys with LPSs of the first type. We mention the study [65] in this regard, the authors of this investigation having observed that the structure of one-domain long-period alloys based on the L1_2 superstructure consists of a mixture of domains of different sizes. If the domains are regularly spaced, then their distribution function will have a sharp profile. The distribution will be diffuse in character if the domains are randomly distributed.

The ANNNI model (axial next nearest-neighbor Ising) model has recently received a lot of attention [66, 67], this being a thermodynamic approach based on the notion of competition between interactions of the nearest and next nearest-neighbors along the modulation direction. The model has been used quite extensively [66-88], including for the purpose of examining problems concerning the formation of polytypic structures [79-82]. The study [83] is interesting in regard to the possibilities of the model in explaining the structure and behavior of alloys with LPSs. The authors of [83] compared the Cato model [18] and a model based on the statistical theory of effective pair interaction (i.e., the ANNNI model). They came to the conclusion that alloys of the types Ag_3Mg , Au_3Zn , and Cu_3Al (in our classification, these are alloys with LPSs of the second type) are adequately represented in the Fujiwara model and can be described physically by the ANNNI model. The model cannot be used for alloys of the types Cu_3Pd , Cu_3Pt , and CuAu (with LPSs of the first type). The transition between proportionate and

disproportionate structures is more complex in these alloys than in the ANNNI model and has many special features [83]. The given model began to later be used intensively to examine LPSs [84]. It is particularly interesting to examine the use of this model for alloys of the system Ti–Al [85], due to the specific temperature dependence of the mean long period of the disproportionate phase. Since it is necessary to know the APB distribution function, the latter was found in the form of a smoothed rectangular distribution for Al_3Ti in [85]. It was also established that this function is an accurate reflection of structures with APBs for Al_3Ti within the temperature region in which the disproportionate phase exists. Proceeding on the basis of the available information, the authors of [69, 86] determined that the ANNNI model describes the temperature- or entropy-induced formation of long-period superstructures in A_3B alloys of the Al_3Ti type on the basis of competing short-range forces. They also determined that the model makes it possible to describe the behavior of binary alloys with a modulated structure [87] and, in the mean-field approximation, describe disproportionate and proportionate structures with modulation in one, two, or three of the main directions of the cubic lattice. A qualitative analysis of the relative stability of long-period superstructures $\text{L1}_2(\text{M})$ based on the Gorsky–Bragg–Williams (GBW) model showed [89] that the GBW model becomes equivalent to the ANNNI model – which employs effective parameters of the interaction between layers of two-component planes.

The authors of [88] studied the effect of the form of the potential on the relative stability of phases with an LPS in the GBW approximation. They established the following general law by minimizing the free energy for phases with different LPSs: the wave vector changes in the direction of the potential minimum (with allowance for temperature) and the stability of the complex phases increases with an increase in the depth of this minimum.

Proceeding on the basis of the successes achieved with the ANNNI model, it can be assumed that the formation of LPSs of the second type is connected with competing interactions. Thus, when examining the long-period states of alloys, the traditional theory of ordering should be supplemented by consideration of such interactions. Since the stability of the long-period state of the alloy will be determined by internal energy of a quasi-chemical nature (by the change in the number of bonds of a certain type), we will henceforth refer to LPSs of the second type as "quasi-chemical LPSs." The formation of a disproportionate state in this case will be a consequence of the entropy factor. To some extent, the proposed approach will also make it possible to relate representations of LPSs to the accumulated data on atomic ordering in alloys. Thus, physical representations of the nature of alloys with LPSs of the second type (Al_3Ti , Ag_3Mg , Cu_3Al , etc.) have now been constructed within the framework of the Ising model with allowance for competing interactions. However, the ANNNI model itself, developed originally for ferromagnetic materials, does not (in its traditional form) account for changes in the internal characteristics of the thermodynamic system with variation of the external conditions.

The situation is more complicated in regard to representations of the nature of alloys with LPSs of the first type (alloys of the system Cu–Au, Cu_3Pd , Cu_3Pt , etc.). It can be assumed that their formation and behavior are determined by relaxation processes (lattice modulation or atomic displacements and redistribution of the atoms of the main components or alloying elements). In light of this, LPSs of the first type will henceforth be called "relaxational LPSs." Since the transition in such alloys is in some respects similar to a martensitic (nondiffusional) transformation, atomic displacements are likely to play a greater role. It can be expected that a certain role will be played by the intradomain part, i.e., a certain averaged interaction of the antiphase boundaries. The most probable reason for the stabilization of LPSs of this type is a reduction in the elastic energy of the partially ordered crystal by some mechanism – specifically, as a result of atomic displacements of an optical nature. Indirect proof of this comes from the empirical determination [90] of the importance of the dimensional factor in long-period structures.

The arguments just examined were used as the basis for the representations in [91-120] regarding the formation and behavior of LPSs of the first type. Comparison of the heuristic consequences [91] of the given model and the laws known to govern the behavior and structure of LPSs did not reveal any inconsistencies. To illustrate the model and check the validity of the representations, calculations were performed using a model alloy with a two-dimensional lattice [92-97]. It was shown quantitatively that the proposed hypothesis may be the reason for the stabilization of LPSs. The main factors that facilitate and impede the formation of relaxational LPSs were determined. Relaxational LPSs in alloys with the base superstructures L1_2 and L1_0 were examined in [98-101] as an outgrowth of the representations in order to analyze whether or not the long-period state is more energetically favorable than the base superstructure as a result of relaxation effects in the form of lattice modulation. The studies were conducted at $T = 0$ to exclude the effects of redistribution of the components and the entropy factor. Characteristics of the initial state (the superstructure L1_2 or L1_0) corresponding to the minimum of internal energy were determined for the chosen interaction. Here, special attention was given to cases in which a newly introduced APB unrelaxed by atomic displacements increases the internal energy of the system for all boundary densities, i.e., cases in which, in the

absence of relaxational effects and regardless of domain size, LPSs are unfavorable for the crystal. The dependence of the internal energy of the APBs of a relaxed (by atomic displacements) long-period state on the size of the long period ($P = 2M$), calculated per atom of the alloy $e = e(M)$, has the form of a curve with a minimum. We should mention the special case in which internal energy is within the region of positive values when the dimensions of the antiphase domain M are small. This situation is a result of the increase in the energy of the system that occurs with the formation of LPSs even when relaxation takes place. An increase in the size of the domain M (a decrease in the density of APBs) causes the curve of the given dependence to shift to the region of negative values, i.e., to a region in which the long-period state is energetically favorable compared to the initial state (base superstructure). The minimum on the curve means that, for the given interaction, the long-period state is favorable with a certain size of antiphase domain. It is significant that the energies of domains of different size differ negligibly in the region of the minimum. Thus, at temperatures different from zero, we should expect the alloy to be in a state that is mixed with respect to M .

The following has been determined in regard to the structure of equilibrium (relaxed) antiphase domains. The formation of an LPS on the basis of the $L1_2$ superstructure results in an increase in the lattice constant along the long period – similar to the situation in Au_3Cd [102] and $CuAuII$ [103] – and compression in the directions normal to this period.

The picture is more complicated in LPSs based on an $L1_0$ superstructure. First of all, there are three different values of the lattice parameter. The transition to the long-period state is accompanied by a reduction in the degree of tetragonality in planes perpendicular to the long period and an increase in tetragonality in planes containing the long-period direction. In other words, an overall expansion of the lattice takes place along the long period, as has been observed experimentally in $CuAuII$ [103].

The structure of the perturbation region near periodic APBs is analogous to that for LPSs with the base superstructures $L1_2$ and $L1_0$: the "lighter" (smaller) atoms are displaced farther from the APB, while the "heavier" (larger) atoms are moved toward it. This conclusion agrees qualitatively with the pattern observed experimentally in Au_3Cd [102] and $CuAuII$ [103]. The region of local singularities (intensive atomic displacements) envelops the 2-3 atomic planes closest to the APB. The perturbations amount to 1-3% of the atomic spacing in the atomic plane closest to the APB. The displacements rapidly decrease with distance and nearly vanish by the third plane. The size of the perturbation region and the magnitude of the perturbations remain nearly constant with a change in the size of the domain. These structural features were later substantiated by independent calculations performed for one-domain APBs [102, 103].

Thus, two important facts have been established. First and most important, in alloys with an LPS of the relaxational type, relaxational effects in the form of lattice modulation ensure that this LPS will be energetically more favorable than the initial superstructure ($L1_2$ or $L1_0$, for example) even at $T = 0$. Secondly, the structure and dimensions of the regions of atomic displacement near the periodic APBs of relaxational LPSs are no different from the corresponding regions of single APBs; the largest atomic displacements are localized near each APB and rapidly decrease with increasing distance from it [104, 105].

This approach has been used to examine a conceptually important aspect of the behavior of alloys with relaxational LPSs — their behavior when the external conditions of the system are varied [106-120]. Most often, the emphasis has been on the effect of temperature on the stability and structural characteristics of the alloys [106-114, 120].

Within the framework of the given representations, the effect of temperature is linked with a competition between two factors: the temperature dependence of the energy of the APBs; the temperature dependence of the resulting elastic stresses. The author of [108, 120] examined the case of the formation of LPSs within a certain temperature interval near the order–disorder transition (T_c) and studied the effect of temperature on the long period of LPSs, as well as microscopic characteristics of the phases that are formed. The focus of the research was on the redistribution of the components of the alloy. A model alloy of the Cu_3Au type, with one long-period direction, was examined in the investigations. Of special interest is the case when a newly introduced periodic APB increases the free energy of the alloy and the long-period state becomes more thermodynamically favorable due to relaxation processes (atomic displacements and redistributions of the components). It should be noted first of all that an analysis of the characteristics of the order–disorder transition of the model alloy revealed a very slight thermodynamic stimulus to the phase transformation in the neighborhood of T_c , which means that it is possible for ordered and disordered phases to coexist within a certain temperature interval.

Calculations performed for the temperature range below T_c showed the characteristic dependences of the free energy of periodic APBs per atom of the alloy on the size of the antiphase domain M . At low temperatures, a phase without periodic APBs turns out to be more thermodynamically favorable in any case. With an increase in temperature, the free energy of an equilibrium (relaxed) APB shifts to the region of negative values, i.e., the region in which an LPS is thermodynamically favorable. Meanwhile, the form of the curve $f = f(M)$ is similar to the case $e = e(M)$ at $T = 0$ K. With an increase in

temperature, the minimum of the curve shifts in the direction of smaller M . Thus, LPSs turn out to be favorable within a certain temperature interval below T_c . With an increase in temperature, the following equilibrium structures are seen: base superstructure – LPS – disordered phase.

Within the temperature interval in which LPSs exist, the presence of the minimum on the curve $f = f(M)$ indicates the possible existence of a state that is mixed with respect to M . This state has a set of equivalent antiphase domains. In this case, the energy factor plays the dominant role in stabilization of the LPSs.

It is useful to examine the microscopic characteristics of an alloy in the long-period state. It follows from a comparison with the case of zero temperatures that the dimensions of the lattice modulation region remain the same in the case of nonzero temperatures. The region of lattice perturbations also tends to remain the same with a change in the size of the antiphase domain. The largest deviations are localized near the APBs and amount to up to 0.6% of the mean interplanar spacing.

It was shown in [104, 105] that at temperatures below T_c , not only does the size of the perturbed region at the APB remain unchanged, but so does the character of perturbation in this region. The main features of the region of perturbation of a single APB are also seen in the case of the periodic alignment of APBs at $T > 0$ K.

Let us examine the effects connected with redistribution of the components of the alloy, since a complex pattern of atom distribution is seen in the equilibrium long-period state. A wall composed of atoms of one of the components is formed at the APB. It should be noted that if the atomic plane closest to the APB contains points that are regular for the atoms of the given species, then there will be a split within this plane with respect to both the probabilities of substitution of atoms and the positions of the atoms. This situation is qualitatively consistent with that seen experimentally in Au_3Cd [102]. A transition to the long-period state leads to a situation in which, along with the formation of segregates of one of the components on the APB, there is a change in the degree of ordering inside the domain. The largest deviations from the initial value are seen in the neighborhood of the APB, the magnitude of these deviations depending on the size of the domain [108, 120]. It is known from experimental data that with a deviation from stoichiometry in $Cu-Au$ alloys, excess atoms are concentrated near APBs, while the parameter characterizing long-range order deviates from the mean in this region [121].

An analysis of the characteristics of antiphase domains has shown that they change slightly against the background of general disorder as temperature increases.

Calculations of the equilibrium distribution function of domain size $\rho = \rho(M)$ showed that it is unimodal. With an increase in temperature, the maximum is shifted to the region of smaller values and becomes less pronounced.

The calculated temperature dependence of mean domain size is qualitatively close to the analogous dependence obtained experimentally for alloy $Cu - 32.2$ at. % Au in the one-phase region of Cu_3Au [122].

Using information on the microstructure of antiphase domains and the distribution function, we constructed patterns comparable to those obtained in full-scale structural investigations. For example, we were able to construct the pattern of x-ray scattering by an ordered long-period phase [109, 114]. The superstructure reflections (010), (110), and (210) turned out to be split, which reflects the pattern observed experimentally. The splitting was symmetrical relative to the position of the superstructure maximum for the initial phase without an APB, but the split doublet was asymmetric with respect to intensity. An analysis showed that modulation of the lattice and redistribution of the atoms of the components do not decisively impact the character of distribution of intensity. The main role in forming the pattern of intensity distribution is played by the presence of a long period. As was shown, an increase in temperature is not accompanied by any significant changes in the character of distribution of intensity. There is only some increase in the background and a reduction in the height of the peaks.

Thus, an equilibrium long-period structure is realized within a certain temperature interval in the following sequence of states: base superstructure – LPS – disordered structure. The LPS is more thermodynamically favorable because of a reduction in the internal energy of the alloy brought about by relaxation processes. Configurational entropy plays a secondary role. The temperature dependence of the long period is determined by the temperature dependence of the energy of the APBs.

The dimensions of the lattice perturbation region at nonzero temperatures are basically the same as at absolute zero, as is the character of the relative atomic displacements. An important difference is the local change in composition and the degree of long-range order in the immediate vicinity of a periodic APB. Even in a binary alloy, there is a high degree of segregation at the antiphase boundary.

At temperatures near T_c , the long-period state is realized in the form of an ensemble of domains of different sizes with similar energies. The size distribution function of the domains is unimodal. Its maximum becomes less distinct with an increase in temperature and the values at the maximum decrease. The mean size of the antiphase domain decreases with an increase in temperature, while the variance and standard deviation increase.

We also examined the combined effect of temperature and hydrostatic pressure on the formation of relaxational LPSs [115-118]. It was found that the presence of external hydrostatic pressure leads to narrowing of the temperature interval in which LPSs of this type exist. The interval is shifted in the direction of higher absolute temperatures.

The dimensions of the lattice perturbation region and the character of the relative displacements of atoms in this region remain nearly unchanged with a change in the external conditions (temperature and pressure). Thin interlayers (1-2 atomic planes) are seen at the APB within the temperature interval in which relaxational LPSs exist, with local jumps in composition and the degree of long-range order occurring in these layers. The presence of pressure fundamentally alters the type of segregating element and the direction of the jump in the order parameter. In the case of the application of external pressure, the antiphase boundary is enriched by smaller-radius atoms, and significant atomic disordering occurs near the boundary.

LONG-PERIOD STRUCTURES IN ALLOYS WITH A BCC LATTICE

There is a wide range of alloys which have a bcc lattice in the high-temperature state that, upon cooling, orders to a structure of the B2 type. A further reduction in temperature is accompanied by a substitutional transition in alloys, such as TiNi, CuZn, and AuCd, that are near equiatomic composition. There are several indications that such transitions occur in more complex superstructures rather than in B2. Diffraction effects corresponding to structures with a tripled period along the cubic axes and a reduction in symmetry to trigonal (rhombohedral) are seen in the pre-transition states. One explanation offered for such effects is the formation of a specific superstructure characterized by the alternation of $\{111\}$ planes in one of the directions $\langle 111 \rangle$ in the form (A) (A) (A) (B) (B) (B) – in contrast to (A) (B) (A) (B) for B2. Here, (A) and (B) denote crystallographic planes with the points occupied mainly by A and B atoms, respectively [123-126]. Wang's hypothesis regarding a specific rhombohedral structure remains unexplored, since the attention of researchers has been focused exclusively on the study of displacement waves.

Structures in which the period has increased several-fold are regarded as "long-period" states in relation to the base superstructure B2. Assuming that the nature of the formation of such states is analogous to the nature of LPSs in alloys with an fcc lattice, we can examine "long-period" states of both the quasi-chemical and the relaxational type.

Structures of the Quasi-Chemical Type. It was shown in [127, 128] that, analogous to the Wang superstructure, several nontraditional superstructures having a tripled period along the axes of the initial cubic lattice can be constructed. For nonstoichiometric compositions, there are several dozen variants of occupation of the points of Wang-type superstructures by excess (compared to the stoichiometric case) atoms of components A or B.

An analysis of the diagrams of the main states (by which we mean the states of the system that are energetically equilibrium states at $T = 0$ K) established the most realistic region of existence of Wang-type superstructures in the energy-parameter state [128, 129]. Several $T-c$ constitution diagrams were later constructed [104].

The completed thermodynamic analysis confirmed that Wang-type superstructures are energetically and thermodynamically favorable within a very broad range of values of the parameters characterizing interatomic interaction. Here, it turned out that a wide range of superstructures of the given type that are energetically similar is possible.

Possibility of Realization of a Columnar Structure of the Relaxational Type. An evaluation was made of the possibility of the formation of ordered long-period states of the relaxational type in binary bcc alloys at $T = 0$ K [130, 131]. Static displacements of atoms from their ideal positions were examined as relaxation processes that stabilize the long-period state. Since there are no references to experimental observations of such structures, the investigation is necessarily of a predictive nature.

We examined the thermodynamic feasibility of the formation of a columnar structure due to the formation of two systems of periodically intersecting APBs $1/2 [111](1\bar{1}0)$ and $1/2 [\bar{1}11](101)$ in a model alloy of equiatomic composition with the base superstructure B2. Anti-phase boundaries of the given orientation were chosen in connection with their low energy of formation. It can be expected from this that relaxational effects will make it possible to stabilize the equilibrium APBs.

The study was conducted with the same approximations and the same approach used in the case of an fcc lattice. We calculated the dependence of defect internal energy on domain size for antiphase columnar structures. It was found that for the given interaction, the energy of the newly introduced unrelaxed defect is within the region of positive values, i.e., a defect should not be realized without relaxational effects. The energy surface of the relaxed equilibrium defect is characterized by the presence of a minimum at certain values of the long period. This means that the formation of a columnar equilibrium antiphase structure of the relaxational type is quite possible from a thermodynamic viewpoint. The analysis also revealed that

the character of the lattice perturbations from a periodic APB and the dimensions of this region are qualitatively consistent with the results obtained from calculations performed for a single APB of the given type in a CuZn alloy [132].

Thus, we can make the following conclusions:

1. A detailed analysis of the structural features and behavior of ordered alloys with a long-period structure indicates the presence of two fundamentally different groups: disproportionate LPSs (CuAuII, Cu₃AuII, Au₃CuII, CuAu—ZnII, one- and two-dimensional LPSs in Cu₃Pd and their analogs); rational LPSs (Ag₃Mg, Al₃Ti, Cu₃Al(α'') and their analogs). It follows from the analysis that the formation and behavior of LPSs in alloys of the first group is determined by relaxation processes; in the second group, the formation of such structures is related to the specifics of interatomic interaction.

2. In the first group of alloys (relaxational LPSs), the stabilization of equilibrium periodic APBs is determined by relaxation processes and is realized only when the gain in relaxation energy is greater than the small increase in the energy of the system that accompanies the formation of APBs due to the formation of high-energy atomic bonds. Long-period structures of the given type may be stabilized by lattice modulation, redistribution of atoms of the components, or their combinations. Since the external conditions of the system have a significant effect on the relaxation properties of the alloy, the existence and nature of the long-period structures are appreciably dependent on changes in the external conditions.

In temperatures differing from absolute zero, the long-period state of the alloy is realized in the form of an ensemble of antiphase domains of different sizes but similar energies. The size distribution of the domains is unimodal. Its maximum becomes less pronounced with an increase in temperature and the values at the maximum decrease.

Local structural features (deviations in composition and the degree of long-range order, lattice modulation, etc.) are seen near periodic structural defects (periodic antiphase boundaries). According to theoretical estimates, the size of the region in which these features are located spans 2-3 atomic planes and remains nearly constant with a change in domain size.

3. In the second group of alloys (quasi-chemical LPSs), the deciding role in the realization of LPSs is competitive interaction in different coordination spheres, assuring a gain of energy in the system in the presence of APBs. The formation of LPSs of the given type should be expected within a broad range of energy parameters. Here, the low-temperature phase is a long-period (long relative to the base superstructure) superstructure: D0₂₂, D0₂₃, etc. In this case, long-range interaction plays the deciding role: increasingly distant atomic interactions exert the decisive effect as cell size increases in the superstructure that is formed.

4. A thermodynamic analysis of Wang-type superstructures within the framework of representations on the quasi-chemical nature of their formation (quasi-chemical LPSs in bcc alloys) shows that they are energetically and thermodynamically favorable within a broad range of values of the parameters that characterize atomic interaction. Here, a wide range of energetically similar Wang-type superstructures may be formed.

CONCLUSION

This article has examined the conditions of formation and behavior of ordered binary alloys and compounds with periodic or quasi-periodic planar equilibrium structural defects. The elements with the lowest energies of formation — antiphase boundaries — can be chosen as such defects, but the proposed models and approaches are applicable to a broader range of both planar and point defects.

We should point out that the investigations discussed here often make no pretense of being comparable to the experimental data, since the stated goal is to develop a physical conception of alloys of the given type. The alloys that were examined (relaxational and quasi-chemical LPSs) are only the extreme cases of a number of alloys grouped together according to characteristics. The system Cu—Pd can be taken as an example. Long-period structures of the relaxational type are realized in alloys of this system that have a composition close to Cu₃Pd. The LPSs become increasingly quasi-chemical in nature with an increase in the content of Pd, as is evidenced by the formation of mixtures of proportionate structures beginning at a certain concentration of Pd.

For the most part, researchers examined new models that link the formation of relaxational LPSs with cooperative behavior among atoms in planes filled to different extents. However, the application of the approaches that were developed is undoubtedly broader, since they also make it possible to consider cases in which the degree of occupation is the same but the atomic interaction is anisotropic.

It should be emphasized especially that the key element in the stabilization of relaxational LPSs is the internal region of the nondefective space, not the region of structural perturbations in the neighborhood of the defect. Although the changes

in this space are not as great, they are sufficient for thermodynamic realization of the long-period state. In essence, the sections between the APBs reflect the average interaction of the APBs themselves. It is significant that the resulting changes in the internal energy of the system lead to the formation of relaxational equilibrium LPSs, while changes in entropy play only a secondary role.

The above investigation embraced different interacting structural levels: the atomic level, in the discussion of the internal features of antiphase domains; the microblock (antiphase-domain) level (with the use of data on the atomic level) in the examination of statistical features of an ensemble of domains.

It is also noteworthy that a method was devised for solving modeling problems. The method makes it possible to reconstruct the complete chain of cause-and-effect relationships: physical representations of the nature of LPSs – the energetic and thermodynamic advantageousness of the long-period state – structural features of LPSs at the atomistic level – statistical laws governing an ensemble of antiphase domains – the average characteristics of the system – theoretical calculation of patterns from structural studies (x-ray diffraction patterns, neutron diffraction patterns, etc.). This information can be compared directly with experimental data.

Alloys with long-period structures can be expected to continue to hold great interest as functional materials for a broad range of practical applications. Alloys with quasi-chemical LPSs have excellent prospects for use as structural materials that remain stable within a broad range of temperatures and loads.

REFERENCES

1. M. A. Krivoglaz and A. A. Smirnov, Theory of Ordered Alloys [in Russian], Fizmatgiz, Moscow (1958).
2. A. A. Smirnov, Molecular-Kinetic Theory of Metals [in Russian], Nauka, Moscow (1966).
3. A. A. Smirnov, Theory of Interstitial Alloys [in Russian], Nauka, Moscow (1979).
4. A. A. Smirnov, Metallofizika., **6**, No. 5, 18-23 (1984).
5. A. A. Smirnov, Generalized Theory of the Ordering of Alloys [in Russian], Naukova Dumka, Kiev (1986).
6. P. S. Clapp, Ordered Alloy, Publishing Division, N.Y. (1970), pp. 25-39.
7. H. Sato and R. S. Toth, Alloying Behavior and Effects in Concentrated Solid Solutions, Acad. Press, N. Y., No. 9 (1963), pp. 295-419.
8. J. Villain, J. Phys. Radium., **23**, 861-873 (1962).
9. S. Ogawa, Order-Disorder Transformations in Alloys, Springer, N. Y. (1974), pp. 240-264.
10. Yu. M. Gufan, Structural Phase Transformations [in Russian], Nauka, Moscow (1982).
11. Yu. M. Gufan and V. I. Torgashev, Fiz. Tverd. Tela, **23**, 1129-1135 (1981).
12. L. William McMillan, Melting, Localization, and Chaos: Proc. 9 Midwest Solid State Theory Symp., Argonne, Nov. 2-3, 1981. N. Y. (1982), pp. 111-114.
13. M. A. Krivoglaz, Fiz. Met. Metalloved., **8**, No. 5, 648-666 (1959).
14. M. A. Krivoglaz, Diffuse Scattering of X-rays and Neutrons on Fluctuational Discontinuities in Nonideal Crystals [in Russian], Naukova Dumka (1984).
15. D. A. Vul' and M. A. Krivoglaz, Metallofiz., **7**, No. 3, 3-12 (1985).
16. D. A. Vul', Fiz. Met. Metalloved., **65**, No. 1, 66-73 (1988).
17. M. Avignon and B. K. Chakraverty, Phase Transform. Solids. Symp., Maleme-Chania, Crete, June-July, 1983. New York (1984), pp. 259-262.
18. H. Sato and R. S. Toth, Phys. Rev., **124**, 1833-1947 (1961).
19. N. F. Mott and H. Jones, The Theory of the Properties of Metals and Alloys, Oxford Univ. Press, London (1936).
20. J. C. Slater, Phys. Rev., **84**, 179-181 (1951).
21. H. Sato and R. S. Toth, Phys. Rev., **127**, 469-484 (1962).
22. R. S. Toth and H. Sato, J. Appl. Phys., **33**, 3250-3258 (1962).
23. J. E. Nicolas, Proceedings Phys. Soc. (London), **A66**, 201-208 (1953).
24. H. Sato and R. S. Toth, Phys. Rev. Lett., **8**, 239-241 (1962).
25. M. Tachiki and K. Teramoto, J. Phys. Chem. Solids, **27**, 335-348 (1966).
26. S. Kubo and K. Adachi, J. Phys. Soc. Jpn., **35**, 776-784 (1973).
27. M. Tachiki and S. Maekawa, J. Phys. Soc. Jpn., **28**, No. 2, 375-379 (1970).

28. V. M. Dement'ev and E. V. Kozlov, *Izv. Vyssh. Uchebn. Zaved., Fiz.*, No. 8, 21-28 (1973).
29. V. M. Dement'ev and E. V. Kozlov, *Izv. Vyssh. Uchebn. Zaved., Fiz.*, No. 6, 30-33 (1974).
30. E. V. Kozlov, V. M. Dement'ev, V. N. Emel'yanov, et al., *Metallofiz.*, **52**, 35-40 (1974).
31. D. A. Vul' and M. A. Krivoglaz, Preprint IMF 17.81, Kiev (1981).
32. D. A. Vul' and M. A. Krivoglaz, *Fiz. Met. Metalloved.*, **51**, 231-245 (1981).
33. D. A. Vul' and M. A. Krivoglaz, *Fiz. Met. Metalloved.*, **52**, 1127-1140 (1981).
34. D. A. Vul' and M. A. Krivoglaz, *Fiz. Met. Metalloved.*, **55**, 869-881 (1983).
35. D. A. Vul' and M. A. Krivoglaz, *Fiz. Met. Metalloved.*, **4**, No. 6, 3-12 (1982).
36. M. A. Krivoglaz, *Theory of the Scattering of X-rays and Thermal Neutrons by Real Crystals* [in Russian], Nauka, Moscow (1974).
37. M. A. Krivoglaz, *Zh. Eksp. Teor. Fiz.*, **84**, No. 1, 355-369 (1983).
38. D. A. Vul', M. A. Krivoglaz, and O. V. Martynenko, *Fiz. Tverd. Tela*, **30**, No. 11, 3417-3425 (1988).
39. M. A. Krivoglaz, *Electronic Structure and Electronic Properties of Metals and Alloys* [in Russian], Kiev (1988), pp. 3-39.
40. N. M. Matveeva and E. V. Kozlov, *Ordered Phases in Metallic Systems* [in Russian], Nauka, Moscow (1989).
41. M. Guymont and D. Gratias, *Phys. Status Solidi A*, **36**, 329-334 (1976).
42. M. Guymont and D. Gratias, *Acta Crystallogr.*, **A35**, 181-188 (1979).
43. D. Watanabe, *Modulated Struct., Int. Conf., Kailua Kona, Haw., 1979. N. Y.* (1979), pp. 229-239.
44. M. Kataoka, *J. Phys. Soc. Jpn.*, **46**, No. 4, 1176-1184 (1979).
45. T. Janssen and J. A. Tjon, *Bulletin of Alloy Phase Diagrams*, **3**, No. 3, 281-287 (1982).
46. K. Schubert, *Crystalline Structures of Two-Component Phases*, Metallurgiya, Moscow (1971).
47. K. Schubert, B. Kiefer, M. Wilkens, and R. Haufler, *Z. Metallkd.*, **46**, 692-715 (1958).
48. K. Schubert, *Z. Naturforsch.*, **14a**, 650-673 (1958).
49. K. Schubert, *Z. Metallkd.*, **53**, 605-632 (1962).
50. K. Schubert, *Trans. Jpn. Inst. Met.*, **14**, 273-280 (1973).
51. H. Jones, *J. Phys. C*, **2**, 760-761 (1969).
52. J. E. Inglesfield, *J. Phys. F*, **2**, 68-72 (1972).
53. R. Kikuchi and H. Sato, *Acta Metall.*, **22**, 1099-1112 (1974).
54. R. Kikuchi and J. Cahn, *Acta Metall.*, **27**, No. 8, 1337-1353 (1979).
55. J. M. Sanchez, S. Eng, Y. P. Wu, and J. K. Tien, "High-Temperature Ordered Intermetallic Alloys II: Symp.", Boston, Mass., Dec. 2-4, 1986. Pittsburgh (Pa) (1987), pp. 57-64.
56. F. Llvét, *J. Phys.*, **50**, No. 19, 2983-2990 (1989).
57. D. C. Chrzan and L. M. Palicov, *Phys. Rev. B*, **40**, No. 12, 8194-8202 (1989).
58. K. Fujiwara, *J. Phys. Soc. Jpn.*, **12**, 7-13 (1957).
59. G. Jehanno and P. Perio, *J. Phys. Radium*, **25**, 966-974 (1964).
60. J. Kakinoki and J. Minagawa, *Acta Crystallogr.*, **A27**, 647-658 (1972).
61. J. Kakinoki and I. Komura, *Acta Crystallogr.*, **19**, 137-147 (1965).
62. J. Minagawa, *Acta Crystallogr.*, **A28**, 307-313 (1972).
63. M. Guymont, D. Gratias, and R. Portier, *Modulated Struct., Int. Conf., Kailua Kona, Hawaii, 1979. N. Y.* (1979), p. 244-246.
64. M. Guymont, R. Portier, D. Gratias, and W. M. Stobbs, *Modulated Struct., Int. Conf., Kailua Kona, Hawaii, 1979. N. Y.* (1979), p. 256-258.
65. N. Kuwano, Y. Tomokiyo, K. Oki, and T. Eguchi, *Phase Transform. Solids, Symp., Maleme—Chania, Crete, June-July, 1983. N. Y.* (1984), pp. 263-268.
66. M. E. Fisher and W. Selke, *Philos. Trans. R. Soc.*, **302**, No. A1463, 1-44 (1981).
67. W. Selke and J. Jeomens, *J. Phys. A*, **16**, No. 12, 2789-2800 (1983).
68. D. De Fontaine and J. Kulik, *Acta Metall.*, **33**, No. 2, 145-165 (1985).
69. W. Selke, *Alloy Phase Stabil.: Proc. Nato Adv. Study Inst., Melans, June 13-17, 1987. Dordrecht etc.* (1989), pp. 205-232.
70. A. I. Ustinov, A. Yu. Gaevskii, A. D. Rud', et al., *Fiz. Met. Metalloved.*, **62**, No. 3, 519-526 (1986).
71. A. I. Ustinov, A. Yu. Gaevskii, A. D. Rud', et al., *Metallofiz.*, **8**, No. 4, 112-114 (1986).

72. A. Yu. Gaevskii and A. I. Ustinov, *Fiz. Met. Metalloved.*, **61**, No. 6, 1064-1071 (1986).
73. E. D. Belokolos and A. Yu. Gaevskii, Preprint IMF 15.88, Kiev (1988).
74. A. Yu. Gaevskii, *Metallofizika*, **9**, No. 4, 92-101 (1987).
75. A. Yu. Gaevskii, Preprint IMF 38.89, Kiev (1989).
76. A. Yu. Gaevskii, *Metallofizika*, **10**, No. 6, 83-86 (1988).
77. A. Yu. Gaevskii, *Metallofizika*, **12**, No. 1, 31-38 (1990).
78. E. D. Belokolos and A. Yu. Gaevskii, *Fiz. Met. Metalloved.*, No. 4, 48-58 (1990).
79. B. I. Nikolin, *Multilayered Structures and Polytypism in Intermetallic Alloys [in Russian]*, Naukova Dumka, Kiev (1984).
80. B. I. Nikolin, *Fiz. Met. Metalloved.*, **45**, No. 1, 110-117 (1978).
81. B. I. Nikolin and S. A. Nefedov, *Metallofizika*, **10**, No. 4, 119-120 (1988).
82. B. I. Nikolin, *Structure of Rheological Machines [in Russian]*, Kiev (1988), pp. 101-132.
83. J. Kulik and D. De Fontaine, *Phase Transform. Solids., Symp., Maleme—Chania, Crete, June-July, 1983*. N. Y. (1984), pp. 225-230.
84. S. C. Moss, *Alloy Phase Stabil.: Proc. NATO Adv. Study Inst., Maleme, June 13-17, 1987*. Dordrecht etc. (1989), pp. 1-4.
85. A. Loiseau, J. Planes, and F. Ducastelle, *Alloy Phase Stabil.: Proc. NATO Adv. Study Inst., Maleme, June 13-17, 1987*. Dordrecht, etc. (1989), pp. 101-106.
86. W. Selke, *Phys. Rep. (Review Section of Phys. Lett.)*, **170**, No. 4, 213-264 (1988).
87. P. Upton and J. Yeomans, *Phys. Rev. B*, **40**, No. 1, 479-492 (1989).
88. G. Ceder, M. De Graef, L. Delaly, et al., *Phys. Rev. B*, **39**, No. 1, 381-385 (1989).
89. B. B. Khaimzon, A. I. Potekaev, and Yu. I. Paskal', *Izv. Vyssh. Uchebn. Zaved., Fiz.*, No. 12, 60-63 (1992).
90. A. A. Boner, T. Ya. Belikanova, V. M. Danilenko, et al., *Phase Stability and Phase Equilibria in Alloys of the Transition Metals [in Russian]*, Naukova Dumka, Kiev (1991).
91. N. S. Golosov and A. I. Potekaev, *Izv. Vyssh. Uchebn. Zaved., Fiz.* (1978). Submitted to VINITI 25.04.78, No. 1411.
92. N. S. Golosov and A. I. Potekaev, *Ordering of Atoms and Its Effect on the Properties of Alloys [in Russian]*, Tomsk (1978), pp. 43-47.
93. A. I. Potekaev and N. S. Golosov, *Summary of Documents of the V All-Union Conference on the Ordering of Atoms and the Effect of Ordering on the Properties of Alloys [in Russian]*, Tomsk (1976), p. 69.
94. A. O. Potekaev and N. S. Golosov, *Handbook: Ordering of Atoms and Its Effect on the Properties of Alloys*, Izd-vo TGU, Tomsk (1978), pp. 43-47.
95. A. I. Potekaev and N. S. Golosov, *Materials of the VI All-Union Conference on the Ordering of Atoms and Its Effect on the Properties of Alloys*, Kiev (1980), pp. 67-71.
96. A. I. Potekaev and N. S. Golosov, *Fiz. Met. Metalloved.*, **46**, 762-771 (1978).
97. A. I. Potekaev and N. S. Golosov, *Fiz. Met. Metalloved.*, **50**, 261-268 (1980).
98. A. I. Potekaev, V. E. Egorushkin, and N. S. Golosov, *J. Phys. Chem. Solids*, **46**, No. 2, 171-174 (1985).
99. A. I. Potekaev, V. E. Egorushkin, and N. S. Golosov, *Izv. Vyssh. Uchebn. Zaved., Fiz.* (1982). Submitted to VINITI 12.05.85, No. 1713.
100. A. O. Potekaev, V. E. Egorushkin, and N. S. Golosov, *Constitution Diagrams of Metallic Systems [in Russian]*, Nauka, Moscow (1982), pp. 20-21.
101. A. I. Potekaev, *Izv. Vyssh. Uchebn. Zaved., Fiz.*, No. 6, 41-45 (1984).
102. M. D. Starostenkov and B. F. Dem'yanov, *Metallofizika*, **7**, No. 3, 105-109 (1985).
103. M. D. Starostenkov and A. N. Yas'kov, *Fiz. Met. Metalloved.*, **60**, No. 5, 1023-1025 (1985).
104. A. I. Potekaev, *Physico-Mathematical Sciences Doctoral Dissertation*, TGU, Tomsk (1993).
105. A. I. Potekaev, *Author's Abstract of Physico-Mathematical Sciences Doctoral Dissertation*, TGU, Tomsk (1993).
106. A. I. Potekaev, *Izv. Vyssh. Uchebn. Zaved., Fiz.* (1984). Submitted to VINITI 21.03.84, No. 1565.
107. A. I. Potekaev and L. D. Bynkova, *Use of Mathematical Methods to Describe and Study Physico-Chemical Equilibria [in Russian]*, Novosibirsk (1985), Pt. 2, pp. 139-142.
108. A. I. Potekaev, *Fiz. Met. Metalloved.*, **61**, No. 2, 254-264 (1986).
109. A. I. Potekaev and V. V. Kulagina, *Izv. Vyssh. Uchebn. Zaved., Fiz.*, No. 12, 61-64 (1989).

110. V. V. Kulagina and A. I. Potekaev, Inter-Institute Symposium: Plane Defects in Ordered Alloys and Intermetallides. Barnaul (1989), pp. 3-8.
111. A. I. Potekaev, *Izv. Vyssh. Uchebn. Zaved., Fiz.* (1989). Submitted to VINITI 14.11.89, No. 6855.
112. A. I. Potekaev, Fundamental Problems of Aging. Development of New Classes of Aging Alloys: Fifth All-Union Symposium on the Aging of Intermetallic Alloys, March 14-16, 1989. Sverdlovsk (1989), p. 103.
113. A. I. Potekaev, Inter-Institute Symposium: Kinetics and Thermodynamics of Plastic Deformation. Barnaul (1990), pp. 19-23.
114. A. I. Potekaev, Inter-Institute Symposium: Kinetics and Thermodynamics of Plastic Deformation. Barnaul (1990), pp. 24-28.
115. L. D. Bynkova and A. I. Potekaev, Inter-Institute Symposium: Plane Defects in Ordered Alloys and Intermetallides. Barnaul (1989), pp. 9-13.
116. L. D. Bynkova and A. I. Potekaev, *Izv. Vyssh. Uchebn. Zaved., Fiz.* (1988). Submitted to VINITI 21.04.88, No. 2364.
117. A. I. Potekaev and L. D. Bynkova, *Izv. Vyssh. Uchebn. Zaved., Fiz.*, No. 12, 28-33 (1989).
118. A. I. Potekaev, *Izv. Vyssh. Uchebn. Zaved., Fiz.* (1989), Submitted to VINITI 19.12.89, No 7479.
119. V. S. Demidenko, A. I. Potekaev, V. I. Simakov, and S. A. Volodin, Structural Phase Transformations in Metallic Systems [in Russian], Izd-vo TGU, Tomsk (1992).
120. A. I. Potekaev, *Phys. Status Solidi A*, **134**, 317-334 (1992).
121. H. Iwasaki and Y. Watanabe, *Modulated Struct., Int. Conf., Kailua Kona, Haw., 1979. N. Y.* (1979), pp. 247-249.
122. H. L. Yakel, *J. Appl. Phys.*, **33**, 2339-2343 (1962).
123. F. E. Wang, S. J. Pickart, and H. A. Alperin, *J. Appl. Phys.*, **43**, No. 1, 97-112 (1972).
124. G. D. Sandroock, A. I. Perkins, and R. F. Heheman, *Metall. Trans.*, **2**, No. 10, 2769-2789 (1971).
125. R. Sinclair and H. A. Mohamed, *Acta Metall.*, **26**, No. 4, 623-628 (1978).
126. V. G. Pushin, V. V. Kondrat'ev, and V. N. Khachin, *Izv. Vyssh. Uchebn. Zaved., Fiz.*, No. 5, 5-12 (1985).
127. B. B. Khaimzon, A. I. Potekaev, and Yu. I. Paskal', *Izv. Vyssh. Uchebn. Zaved.* (1991). Submitted to VINITI 25.05.91, No. 2184.
128. B. B. Khaimzon, A. I. Potekaev, and Yu. I. Paskal', *Izv. Vyssh. Uchebn. Zaved., Fiz.*, No. 9, 91-96 (1991).
129. B. B. Khaimzon, A. I. Potekaev, and Yu. I. Paskal', *Izv. Vyssh. Uchebn. Zaved., Fiz.*, No. 7, 32-37 (1992).
130. A. I. Potekaev and V. E. Egorushkin, *Izv. Vyssh. Uchebn. Zaved., Fiz.*, No. 6, 85-89 (1983).
131. A. I. Potekaev and V. E. Egorushin, *Izv. Vyssh. Uchebn. Zaved., Fiz.* (1986). Submitted to VINITI 11.02.86, No. 983.
132. A. I. Potekaev, M. A. Baranov, and M. D. Starostenkov, *Izv. Vyssh. Uchebn. Zaved., Fiz.* (1988). Submitted to VINITI 25.05.88, No. 4055.