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FORMATION OF INTERMEDIATE ORDERED STATES ON SPINODAL DECOMPOSITION OF ALLOYS

I. K. Razumov UDC 669.112:53.091

A model of diffusion phase transformations in alloys with a tendency toward ordering is suggested. It accounts for the vacancy mechanism of diffusion and the possible competition of the processes of ordering and decomposition. It is shown that the spinodal decomposition into components A and B from a homogeneous initial state may pass through the stage of formation of isolations of the ordered phase, with their stability being qualitatively increased in the region of low temperatures. The growth of colonies on decomposition of a metastable ordered state has been investigated.

Introduction. The physical properties of a substance are closely connected with its phase structure; therefore the theory of the decomposition of alloys is of great interest. The equilibrium thermodynamics of transformations [1, 2] allows one to predict the fractions of precipitates at long holding times. At the same time, the desired properties of a substance are often realized during formation of metastable nonequilibrium structures, which requires the study of the kinetics of transformations. The equations of evolution of a disordered alloy in spinodal decomposition (SD) were suggested by Cahn and Hilard [3], followed by the construction of more consecutive microscopic models [4, 5], including those for ordering alloys [6, 7]. However, usually the processes of ordering and decomposition are considered separately, whereas in real systems they can exist simultaneously. Thus, in [8] a tendency toward ordering in the Au–Fe system has been revealed; in [9] the possibility of ordering in the Ti–V alloy in the region of low temperatures is discussed, the authors dealing in this case with the ordering that originates at intermediate stages of decomposition into disordered phases, i.e., with a fundamentally nonequilibrium phenomenon.

The first theoretical investigation of intermediate ordered states was carried out in [10] in the language of Onsager-type semi-phenomenological kinetic equations. Considered was a system having a local minimum of free mixing energy corresponding to an ordered state at a certain concentration ratio of alloy components. By virtue of the presence of this minimum, the decomposition kinetics presupposes ordering even though the phase equilibrium curve preserves a traditional form typical of a regular solid solution. However, computer modeling by the Monte Carlo method [9] has revealed qualitative differences with the predictions made by that theory. Next, the topic was discussed in [7] from methodical considerations; it was shown that a consecutive microscopic approach based on the fundamental kinetic equation leads to the breakdown of the intermediate ordered state whose picture is similar to the results of modeling in [9]. However, as a whole, the problem has remained insufficiently studied. In particular, the kinetics of spinodal decomposition from a homogeneous initial state with formation of intermediate ordered states has not been studied in the language of consecutive microscopic approaches similar to those used in [7]; the conditions that determine the stability degree of ordered states also remain unclear.

In the present work the kinetics of ordering and decomposition is investigated within the framework of the generalization of the hole gas method [11] that combines the simplicity of presentation with the consistency typical of the microscopic method. It is shown that the spinodal decomposition of some alloys into components A and B may proceed in two stages. First it proceeds with separation of an ordered phase and only subsequently the ordered phase undergoes a further decomposition into components A and B. The kinetics of this process has not only some analogy with the approach of [10] but also some differences and depends substantially on temperature. Also, the results of numerical modeling of the process of decomposition of a metastable ordered phase into components A and B are presented. It is shown that it proceeds according to the mechanism of the growth of lamellar structures, is an activation

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Institute of Quantum Material Science, 62–26 Chelyuskintsev Str., Ekaterinburg, 620107, Russia; email: iraz@k66.ru. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 81, No. 4, pp. 789–795, July–August, 2008. Original article submitted December 12, 2006; revision submitted January 15, 2008.

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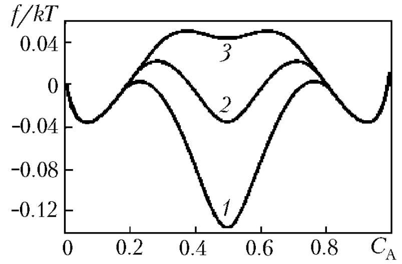

Fig. 1. Free energy of mixing vs. the concentration of the component ($\Psi = 6$): 1) $\Theta > \Psi$; 2) $\Psi = \Theta$; 3) $\Theta < \Psi$.

one, and can be provoked by the distortions of the lattice in the region of the grain boundaries or by the presence of a critical nucleus of the atoms of species A or B in the ordered phase.

1. Formulation of the Model. *1.1. Phase diagram.* We will consider a binary alloy in which ordering is associated with the redistribution of atoms between two equivalent sublattices. In the quasi-chemical approximation [1], the energy of the atoms of species σ = A, B that lie in the sub-lattice n = 1, 2 at the node with a radius-vector $\mathbf{r}$ is determined by the equality

$$E_{\sigma}^{(n)}(\mathbf{r}) = \sum_{\sigma'=\mathrm{A,B}} \sum_{i,m} \varphi_{\sigma\sigma'}^{(nm)}(\mathbf{q}_i)\, C_{\sigma'}^{(m)}(\mathbf{r}+\mathbf{q}_i)\,. \tag{1}$$

Summation is taken over the nodes i of each sub-lattice m = 1, 2. After expansion in terms of $\mathbf{q}_i$ Eq. (1) acquires the form

$$E_{\sigma}^{(n)}(\mathbf{r}) = \sum_{\sigma'=\mathrm{A,B}} \Phi_{\sigma\sigma'}^{0}\left(C_{\sigma'}^{(n)} + R^2 \Delta C_{\sigma'}^{(n)}\right) + \Phi_{\sigma\sigma'}^{+}\left(C_{\sigma'}^{(m)} + R^2 \Delta C_{\sigma'}^{(m)}\right), \quad m \neq n\,, \tag{2}$$

where $\Phi_{\sigma\sigma'}^{0} = \sum \varphi_{\sigma\sigma'}^{(nn)}(\mathbf{q}_i)$; $\Phi_{\sigma\sigma'}^{+} = \sum \varphi_{\sigma\sigma'}^{(nm)}(\mathbf{q}_i)$.

The small parameter R is considered to be a constant. An analysis of the zero-order terms of the expansion in terms of R in (2) allows one to make general inferences on the thermodynamics of transformations. In particular, using the reasoning similar to that applied in [1] and assuming random allocation of atoms in each of the sublattices, for the free energy density of mixing one can easily obtain

$$\frac{f}{kT} = \Theta \eta_{\mathrm{A}} \eta_{\mathrm{B}} + \Psi C_{\mathrm{A}} C_{\mathrm{B}} + \sum_{\sigma,n} C_{\sigma}^{(n)} \ln C_{\sigma}^{(n)}\,, \tag{3}$$

where the dimensionless energies of mixing Ψ and ordering Θ are defined by the sum and difference of the sublattice energies of mixing: $\Psi = (\chi^0 + \chi^+)/(kT)$; $\Theta = (\chi^0 - \chi^+)/(kT)$; $\chi^{0(+)} = 2\Phi_{\mathrm{AB}}^{0(+)} - \Phi_{\mathrm{AA}}^{0(+)} - \Phi_{\mathrm{BB}}^{0(+)}$, whereas the degree of ordering and average concentration in sublattices are: $\eta_\sigma = (C_\sigma^{(1)} - C_\sigma^{(2)})/2$, $C_\sigma = (C_\sigma^{(1)} + C_\sigma^{(2)})/2$. The value of η_σ can be calculated from the Bragg–Williams equation [1, 12]:

$$\frac{(C_\sigma - \eta_\sigma)\,(1 - C_\sigma - \eta_\sigma)}{(C_\sigma + \eta_\sigma)\,(1 - C_\sigma + \eta_\sigma)} = \exp\,(-\,2\Theta\eta_\sigma)\,. \tag{4}$$

Figure 1 presents the graphs of the function $f(C_{\mathrm{A}})$ at different ratios of the parameters $\Psi > 0$ and $\Theta > 0$. Generally, the graph has three minima. The central minimum (C_{A} = 0.5) is absolute provided that $\Theta > \Psi$ (curve 1); in this case the ordered state is stable. At $\Theta = \Psi$ all minima have the same depth (curve 2), which corresponds to conventional equilibrium of the ordered and disordered states. Finally, for $\Theta < \Psi$ (curve 3) the central minimum is local; therefore the ordered states undergo a further decomposition — up to separation into components A and B. When $\Theta < 0$, ordering in an alloy is impossible, whereas with $\Psi < 0$ decomposition into components A and B is impossible.

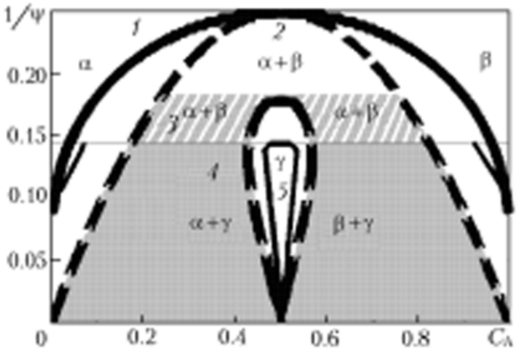

Fig. 2. Phase diagram of an alloy with a tendency toward ordering ($\Psi = 1.2\Theta$): 1) region of a stable alloy; 2) spontaneous decomposition into disordered phases α and β; 3) spontaneous decomposition into phases α and β with formation (at intermediate stages of the kinetics) of an ordered γ phase undergoing further decomposition nonactivative; 4) spontaneous decomposition into a metastable ordered γ phase and a disordered α(β) phase with subsequent decomposition of the γ phase following the mechanism of nucleation of nuclei; 5) metastable ordered states.

Figure 2 presents the phase diagram that corresponds to the case $\Psi > \Theta > 0$, where the tendency toward decomposition dominates over the tendency toward ordering. The stability loss curves denoted by dashed lines were obtained from the condition that $\frac{\delta^2 f}{\delta C_{\mathrm{A}}^2} = 0$ [1]. The curves of phase equilibria (solid lines) were obtained from the condition of equality of the chemical potentials of phases by drawing tangents to the concave portions of the $f(C_{\mathrm{A}})$ curve. In this case, the local minimum of $f(C_{\mathrm{A}})$ is responsible for the appearance of the curves of unstable (metastable) equilibrium, one of which bounds region 5 and the other passes near the upper solid line, which is the curve of stable equilibrium, and terminates at the temperature that corresponds to the apex of region 5.

1.2. Differential equations of the decomposition kinetics. The approach outlined represents the extension of the hole gas method [11] to ordering alloys. The extension of the method to disordered alloys that undergo spinodal decomposition was suggested earlier in [13, 14].

We will identify the concentrations $C_{\sigma(v)}^{(n)}(\mathbf{r})$ of atoms of species σ = A, B and vacancies at the node $\mathbf{r}$ of the sublattice n with the probabilities of finding them at that node. We assume that the occurring diffusion follows the vacancy mechanism and that jumps of atoms are possible between different sublattices and that pair correlations in the distribution of atoms may be neglected (a regular solution [1]). Then the equations of the evolution of concentrations have the form

$$\frac{dC_{\sigma}^{(n)}}{dt}(\mathbf{r}) = \sum_{l=1}^{Z} \omega_{\sigma}^{(m)}(\mathbf{r}+\mathbf{a}_l \to \mathbf{r})\, C_{\mathrm{v}}^{(n)}(\mathbf{r})\, C_{\sigma}^{(m)}(\mathbf{r}+\mathbf{a}_l) - \omega_{\sigma}^{(n)}(\mathbf{r} \to \mathbf{r}+\mathbf{a}_l)\, C_{\mathrm{v}}^{(m)}(\mathbf{r}+\mathbf{a}_l)\, C_{\sigma}^{(n)}(\mathbf{r}) ,$$

$$C_{\mathrm{A}}^{(n)} + C_{\mathrm{B}}^{(n)} + C_{\mathrm{v}}^{(n)} = 1 . \tag{5}$$

Equation (5) by its nature expresses the balance of substances: the change (per unit time) in the probability of detecting atoms of species σ = A, B at the node $\mathbf{r}$ is composed of the probabilities of transition of the atoms of this species from all the nodes of the closets surrounding to that node minus the probabilities of reverse transition. The frequencies of transitions are given by the formulas

$$\omega_{\sigma}^{(m)}(\mathbf{r}+\mathbf{a}_l \to \mathbf{r}) = \omega_{\sigma 0} \exp\left[\left(E_{\sigma}^{(m)}(\mathbf{r}+\mathbf{a}_l) - E_{\sigma}^{s}\right)\big/(kT)\right],$$

$$\omega_\sigma^{(n)}(\mathbf{r}\to\mathbf{r}+\mathbf{a}_l) = \omega_{\sigma 0}\exp\left[\left(E_\sigma^{(n)}(\mathbf{r}) - E_\sigma^{\mathrm{s}}\right)/(kT)\right], \tag{6}$$

with $E_\sigma^{(n)}$ having been defined by Eq. (2); the energy of the atom at the saddle point E_σ^{s} is considered to be a constant for simplicity. Assuming that $C_{\sigma(\mathrm{v})}^{(n)}(\mathbf{r})$ change slowly at distances of the order of a, in Eq. (5) we carry out a series expansion in $\mathbf{a}_l$ and write out the equation of evolution of η_σ and C_σ restricting ourselves to the first nonvanishing terms:

$$\frac{d\eta_\sigma}{dt} = \frac{2}{a^2}\left(\omega_\sigma^{(2)}C_\sigma^{(2)}C_\mathrm{v}^{(1)} - \omega_\sigma^{(1)}C_\sigma^{(1)}C_\mathrm{v}^{(2)}\right), \quad \frac{dC_\sigma}{dt} = -\nabla\mathbf{J}_\sigma\,; \tag{7}$$

$$\mathbf{J}_\sigma = \frac{Za^2}{4}\sum_n \omega_\sigma^{(n)}\left[C_\sigma^{(n)}\nabla C_\mathrm{v}^{(m)} - C_\mathrm{v}^{(m)}\nabla C_\sigma^{(n)} - C_\sigma^{(n)}C_\mathrm{v}^{(m)}\nabla E_\sigma^{(n)}/(kT)\right], \quad n\neq m\,; \tag{8}$$

$$\omega_\sigma^{(n)}(\mathbf{r}) = \omega_{\sigma 0}\exp\left[\left(E_\sigma^{(n)}(\mathbf{r}) - E_\sigma^{\mathrm{s}}\right)/(kT)\right]. \tag{9}$$

From Eq. (7) it is seen that the ordering is a fast process as compared to diffusion. Therefore one may use the approximation of the locally equilibrium ordering by calculating the value of η_σ that corresponds the local concentration C_σ. In this case $\omega_\sigma^{(2)}C_\sigma^{(2)}C_\mathrm{v}^{(1)} = \omega_\sigma^{(1)}C_\sigma^{(1)}C_\mathrm{v}^{(2)}$, whence, with consideration for Eq. (1), we obtain the Bragg–Williams equation (4). The condition of transition from a disordered state to an ordered one can be represented as the limit $|\eta_\sigma| \to 0$ by expanding Eq. (4) into a series in η_σ, and it has the form $1-\Theta C_\mathrm{A}C_\mathrm{B} = 0$; the condition $\Theta = 4$ determines the critical temperature of the ordering. The maximum ordering $\eta_\sigma = \pm 1/2$ is attained when $T\to 0$ and $C_\sigma = 1/2$.

We will rewrite Eq. (8) in the approximation of locally equilibrium ordering and local equilibrium of vacancies $\mathbf{J}_\mathrm{v}\to 0$, $J_\mathrm{A}+J_\mathrm{B}\approx 0$, having selected, for the sake of definiteness, that σ = A and n = 1:

$$\mathbf{J}_\mathrm{A} = \frac{Za^2\omega_\mathrm{A}^{(2)}\omega_\mathrm{B}^{(2)}C_\mathrm{A}^{(2)}C_\mathrm{B}^{(2)}C_\mathrm{v}^{(1)}}{2\left(\omega_\mathrm{A}^{(2)}C_\mathrm{A}^{(2)}+\omega_\mathrm{B}^{(2)}C_\mathrm{B}^{(2)}\right)}\nabla\left[\ln\left(\frac{C_\mathrm{B}^{(1)}}{C_\mathrm{A}^{(1)}}\right)+\frac{E_\mathrm{B}^{(1)}-E_\mathrm{A}^{(1)}}{kT}\right], \tag{10}$$

where the expression for the gradient is expanded with the use of Eq. (2):

$$\nabla\left[\ln\left(\frac{C_\mathrm{B}^{(1)}}{C_\mathrm{A}^{(1)}}\right)+\frac{E_\mathrm{B}^{(1)}-E_\mathrm{A}^{(1)}}{kT}\right]$$

$$= -\left[\left(1-\Psi C_\mathrm{A}^{(1)}C_\mathrm{B}^{(1)}\right)\nabla C_\mathrm{A} + \left(1-\Theta C_\mathrm{A}^{(1)}C_\mathrm{B}^{(1)}\right)\nabla\eta_\mathrm{A} - R^2 C_\mathrm{A}^{(1)}C_\mathrm{B}^{(1)}\nabla\left(\Theta\Delta\eta_\mathrm{A}+\Psi\Delta C_\mathrm{A}\right)\right]\Big/\left(C_\mathrm{A}^{(1)}C_\mathrm{B}^{(1)}\right). \tag{11}$$

The first term in (11) is attributable to the ascending diffusion on decomposition into disordered phases; the second term — to the decomposition with separation of an ordered phase. The terms of the order of R^2 are needed for describing the evolutions of concentrations in the region of interphase and antiphase boundaries and have a traditional form [3, 4, 13, 14].

2. Kinetics of Transformations: the Results of Numerical Simulation. Investigation of the kinetics of decomposition from a homogeneous initial state with small Gaussian fluctuations of the composition was carried out by numerical solution of Eq. (7), using the standard Runge–Kutta method to represent Eqs. (10) and (11) for the flow on a two-dimensional grid $L\times L$. It was assumed that the distributions of concentrations are mirror-symmetric relative to the boundaries of the considered quadratic region. For η_σ locally equilibrium values obtained according to Bragg–Williams from Eq. (4) were used; for the concentration of vacancies it was adopted that $C_\mathrm{v}^{(1)}$ = const. In Figs. 3–6 for sublattices 1 and 2 there correspond staggered pixels. In this case, the concentrations of the component A in each of the sublattices are represented by gradients of gray color. Thus, the disordered regions are colored homogeneously,

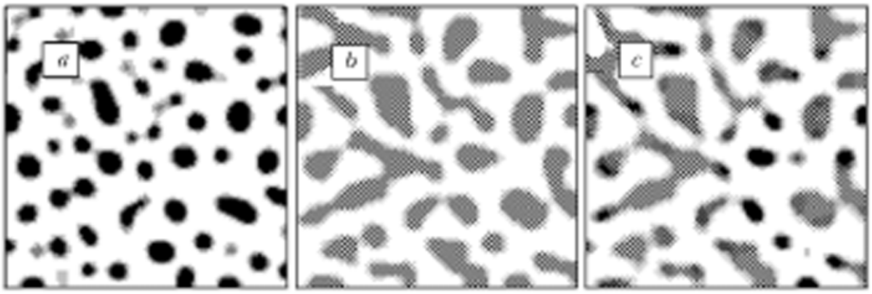

Fig. 3. Characteristic pictures of the wave stage of alloy decomposition from a homogeneous initial state with small Gaussian fluctuations ($C_{A0} = 0.3$, $L = 100R$, $\tau = 0.25$): a) decomposition into α- and β phases at $\Theta = 0$, $\Psi = 7$; b) decomposition into γ- and β-phases at $\Theta = 7$, $\Psi = 5$; c) intermediate ordering on decomposition into α- and β phases at $\Theta = 5$ and $\Psi = 7$.

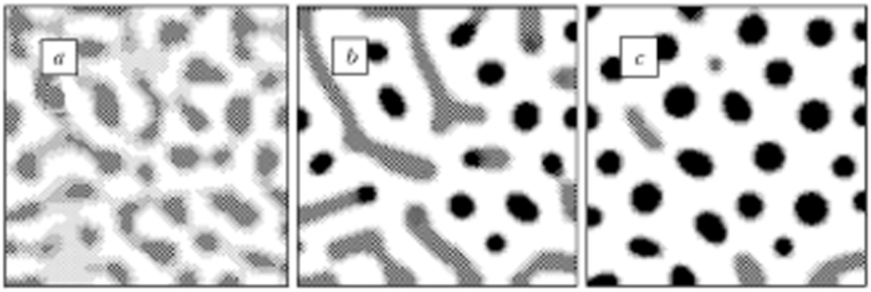

Fig. 4. Kinetics of spinodal decomposition of an alloy with a tendency toward ordering from a homogeneous initial state with small Gaussian fluctuations ($C_{A0} = 0.3$, $L = 100R$, $\Theta = 5$, $\Psi = 6$): a) $\tau = 0.25$; b) 1.1; c) 2.2.

whereas in the ordered regions the cell structure of imaging is manifested. The time τ is given in the units of $Z(\omega_{A0} + \omega_{B0})C_v^{(1)}(a/L)^2 t/2$.

The calculations show that the decomposition of an alloy proceeds following one of three types depending on the relationship between the energies Ψ and Θ. When $\Psi > 4 > \Theta$, there is decomposition into disordered α- and β phases (Fig. 3a). When $\Theta > \Psi$, $\Theta > 4$ there occurs decomposition into the ordered γ phase and disordered α(β) phase (Fig. 3b). When $\Psi > \Theta > 4$, the evolution of the system may pass through a stage of decomposition into the α(β)- and γ phases, after which the ordered phase also undergoes decomposition (Fig. 3c), and the process continues up to complete separation into α and β, i.e., the ordering appears at the intermediate stages of the kinetics.

The degree of stability of intermediate ordered states depends on temperature. If the parameters of an alloy lie in the hatched region 3 of the phase diagram (see Fig. 2), then the γ phase undergoes a further decomposition without activation (Fig. 4). However, on decrease in temperature the parameters of the alloy are displaced into the darkened region 4 on decomposition from which the attainment of metastable equilibrium of the ordered and disordered phases is possible. Therefore, a further decomposition is possible only by the mechanism of the formation of nuclei. The non-active decomposition $\alpha + \gamma$ in region 4 of the phase diagram accompanied by an increase in the separation of the phase β at the center of the region considered is presented in Fig. 5. This separation brought into the initial state entirely absorbs the γ phase at long holding times.

In region 5 (see Fig. 2) the homogeneous alloy is ordered and stable against small fluctuations of composition; however, its decomposition can be activated either by the nuclei of the α(β) phases introduced into the initial state or by the boundaries of grains. Figure 6 shows the growth of the colony from the grain boundary near which (in the region of width $2R$) the ordering energy Θ is lowered. Such a situation can be implemented, for example, in the alloys that were subjected to intense plastic deformation and the lattice of which is heavily distorted and the thermodynamic properties near the boundaries of grains were changed [15]. As a result of the development of the wave stage of decomposition, a chain of equidistantly located isolations of the α- and β phases is formed along the boundary;

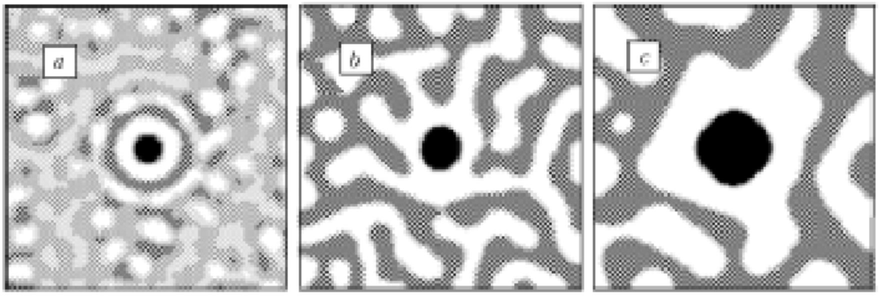

Fig. 5. Kinetics of spinodal decomposition of an alloy with a tendency toward ordering from a homogeneous initial state with small fluctuations and separation of the α phase at the center (C_{A0} = 0.3, L = 100R, Θ = 6.5, Ψ = 7.8): a) τ = 0.25; b) 1.5; c) 8.

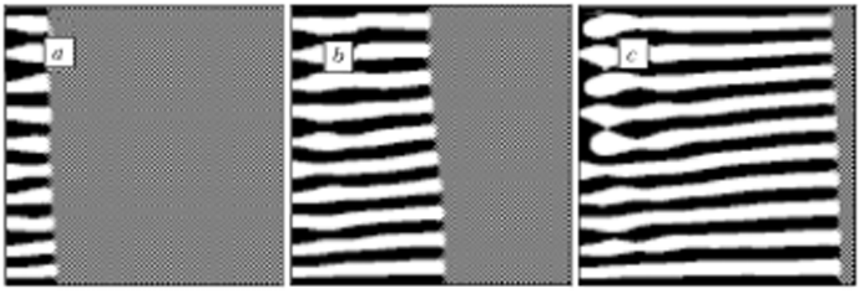

Fig. 6. Growth of a colony from the grain boundary on decomposition of a metastable ordered phase provoked by a 40%-reduction in the energy of ordering Θ in the boundary region of width 2R (L = 200R, C_{A0} = 0.5, Ψ = 6, Θ = 5): a) τ = 1; b) 2, c) 5.

thereafter they grow into the bulk of the grain in the form of parallel lamels of identical width. At the developed stages there occur ageing and destruction of lamels. Calculations show that at the higher temperatures that correspond to region 3 of the phase diagram (see Fig. 2), the formation of lamellar microstructures on decomposition of the metastable γ phase can also be induced by the isolations of the α(β) phases in the bulk of the grain. In such a case there occurs a kind of autocatalysis, so that the isolations of the α phase favor the formation of isolations of the β phase in its vicinity.

3. Discussion of Results. The model of the decomposition of a binary alloy proposed earlier [13, 14] has been generalized to the case of solid solutions with a tendency toward ordering. The specific properties of the approach presuppose: a) account for the vacancy mechanism of diffusion by analogy with the "hole gas" method [11] and b) the continuum approximation allowing one to use diffusion equations in partial derivatives similar to the "phase-field" method and the Cahn–Hilliard SD model [3, 5]. The drawback of these equations is the use of many model assumptions (locally equilibrium ordering, local equilibrium of vacancies, a smooth change of concentrations in space, etc.). At the same time, they give a clearer representation than more rigorous approaches [6, 7], are more convenient for numerical analysis as compared to the Monte Carlo method [9, 16], and allow one to make general inferences on the kinetics of transformations in alloys. The region of applicability of the approach is limited, generally speaking, by the class of systems in which the width of the transient interphase region substantially exceeds the interatomic distance (Fe–Al, Ni–Al, Co–Pt, etc.).

Within the framework of the model an analysis of three types of decomposition is possible, with the first two having been studied in detail in [3–7]. However, the third, SD type that takes into account competition of the processes of ordering and decomposition has been inadequately considered earlier. In [10] intermediate ordered states were predicted; however, the solution of Onsager-type equations has not revealed the possibility of simultaneous existence of three phases in the system: A- and B-enriched and an ordered ones. The change in the composition of separations of an ordered phase in [10] occurs as a result of nonactivative disordering. On the contrary, the analysis carried out in the present work shows that the ordering is the result of decomposition into disordered and A- and B-enriched phases, and, moreover, this decomposition requires activation in the region of low temperatures (see Fig. 5). In the region of elevated temperatures, the decomposition of the γ phase proceeds nonactivatively, but it also is controlled by diffusion, since it occurs as a result of the outflow of the basic component into the neighboring disordered phase through the separation surface. This is indicated, e.g., by the fact that finer separations of the ordered phase undergo decomposition in the first place, whereas in large separations the decomposition develops in the portions that have the greatest curvature of the surface.

The results obtained agree with [9], where the incipience of the A- and B-enriched phases from the intermediate ordered state was investigated by the Monte Carlo method. It was shown that the antiphase boundaries protrude at the places of preferable incipience and the existence of three phases, A- and B-enriched and the ordered one, is possible at intermediate stages. It is interesting to note that in the calculations presented for a number of cases a correct morphology of separations appears at developed stages of transformation. In particular, Fig. 6 demonstrates the lamella microstructure appearing on the decomposition provoked by the grain boundary. An analysis of more complex but qualitatively similar phenomena in steels such as perlite transformation (decomposition of the metastable austenite into cementite and ferrite) [17, 18] has an important practical value, since the technical characteristics of steels (rigidity, plasticity, etc.) are greatly determined by the morphology of separations.

Conclusions. The hole gas method of analysis [11] has been extended to ordering alloys undergoing spinodal decomposition. It is shown that at intermediate stages of the kinetics the existence of there phases: A- and B-enriched and an ordered ones is possible. The ordered phase is metastable in the region of low temperatures, so that its decomposition needs activation. The decomposition of an ordered phase can be induced, e.g., by the grain boundary, and then it proceeds following the mechanism of growth of the colony, which consists of parallel lamellas of identical width.

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NOTATION

a, parameter of the lattice, Å; $\mathbf{a}_l$, radius-vector of the nearest neighbor of an isolated atom, Å; C_σ and $C_{\sigma0}$, local sample-average concentrations of atoms of species σ, $0 \le C_\sigma \le 1$ and $0 \le C_{\sigma0} \le 1$; $C_\sigma^{(n)}$ and $C_\mathrm{v}^{(n)}$, local concentrations of atoms of species σ and vacancies in sublattice n, $0 \le C_\sigma^{(n)} \le 1$ and $0 \le C_\mathrm{v}^{(n)} \le 1$; $E_\sigma^{(n)}$ and E_σ^s, energies of the atom of species σ at the sublattice node n and at the saddle point s, eV; f, density of free mixing energy, eV; $\mathbf{J}_\sigma$ and $\mathbf{J}_\mathrm{v}$, fluxes of atoms of species σ and vacancies, m/sec; k, Boltzmann's constant, $8.6 \cdot 10^{-5}$ eV/K; L, size of a sample, Å; N, number of nodes in a sublattice; $\mathbf{q}_i$, radius-vector of the relative position of the lattice node; $\mathbf{r}$, radius-vector of the relative position of a certain point in space, Å; R, effective radius of interaction of atoms, Å; t, time, sec; T, temperature, K; Z, coordination number; α and β, phases enriched with atoms of species A and B, respectively; γ, ordered phase; η_σ, degree of ordering, $-1/2 \le \eta_\sigma \le 1/2$; Θ, dimensionless energy of the ordering of an alloy; τ, dimensionless time; $\varphi_{\sigma\sigma'}^{nm}$, energy of pair interaction of atoms of species σ and σ' located in sublattices n and m, respectively, eV; $\Phi_{\sigma\sigma'}^0$ and $\Phi_{\sigma\sigma'}^+$, energies of interaction of atoms of species σ with its "own" and "another's" sublattice filled with atoms of species σ', eV; χ^0, χ^+, sublattice energies of mixing, eV; Ψ, dimensionless energy of alloy mixing; $\omega_\sigma^{(n)}$, frequency of passage of atoms of species σ from sublattice n, sec^{-1}; $\omega_{\sigma0}$, value of $\omega_\sigma^{(n)}$ for $T \to \infty$, sec^{-1}. Subscripts and superscripts: i, node of sublattice, 1, ..., N; l, number of the closest neighbor of an atom, 1, ..., N; n, m, Nos. of sublattices 1 and 2; s, saddle point; v, vacancy; σ, σ', species of atoms A and B.

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