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EVOLUTION OF ANTIPHASE ORDERED DOMAIN STRUCTURES IN CONFINED BINARY ALLOYS

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An initial boundary value problem with Dirichlet or Neumann boundary conditions is considered. This problem describes evolution of a nonconserved order parameter in binary alloys near the disordered phase. It is shown that the problem has asymptotically oscillating stationary distributions of the order parameter. This oscillation describes so-called antiphase boundaries (APB) in binary alloys. The corresponding phase diagram is constructed. Particularly, it is shown that the temperature is a bifurcation parameter. The stationary antiphase boundaries with a different number of oscillations between the walls confining the sample arise at cooling in binary alloys on long time scales. Further, it is shown that if there is a small parameter of the system, contrast structures are formed, i.e. step-constant asymptotically stationary distributions of APB.
Keywords: binary alloys, antiphase boundaries.

INTRODUCTION

The paper contains analysis of three main aspects of the problem. The first one is the formation of antiphase domain structures from the disordered state (see [1], Photo. 1, described anneal-ageing of an alloy in disordered state). This process was studied by Matsubara (1990) in Fe_3Al, by Allen and Krzanowsky [1985], Park and Allen [1986] with microscopic observation (see references in [1]). For example, Matsubara [1989] observed the process of DO_3 ordering of Fe_3Al, after quenching from $B2$ state. Here it is assumed that small domains are formed randomly within the disordered ($B2$) matrix. It was supposed in the experiments that the domains change their shapes and sizes at the early stage of isothermal ageing. In contrary, we consider the case of asymptotic behavior as time $t \to \infty$, because the strict asymptotics has not been considered in the previous cited paper.

To analyze the process, the corresponding evolution equation has been constructed [1]. The Allen-Cahn partial differential equation of the second order was supplemented with periodic boundary conditions and random initial conditions. At every moment $t>0$, there are oscillating solutions of sinusoidal type (see [1], Fig. 1). This figure describes the evolution of nonconserved order parameter, which models so-called antiphase boundaries (APBs). Thus, we obtain oscillating order parameter distributions of sinusoidal type in the disordered phase at early stage of evolution. But as $t>0$ is large, we obtain (by computer simulation) the step-constant oscillating structures of relaxation type ([1], Fig.2). In mathematics, such structures are called contrast ones (see, for example, [2]).

In the previous papers, the Allen-Cahn equation with periodic boundary conditions has been studied [1]. Here we consider the Dirichlet and Neumann boundary conditions. In the previous papers, random initial conditions were studied with the help of computer simulation. We consider deterministic initial conditions and use the well-known

mathematical result to study of evolution of non-conserved order parameter in confined binary alloys. We show that the typical asymptotic is sinusoidal near the disordered phase. There are also limit distributions of spike-type, if dimensionless diffusion coefficient is small; and limit distributions exist in the form of stationary contrast structures, if there is the transform $t \mapsto t/\varepsilon$, where $\varepsilon>0$ is the small parameter that characterizes spatial-temporal "inhomogeneities" in the binary alloy and describes the thickness of antiphase boundary layers (see, for example, [3, 4]). Further, we introduce the function of the inhomogeneities at the disordered phase $a(x,\varepsilon)$, which changes the amplitude $u(x,t)\equiv 0$ of the disordered phase by the transform $u(x,t) \mapsto u(x,t) - a(x,\varepsilon)$. Coordinates of the front of phase transition can be established by the coordinates of the intersection of $u(x,0,\varepsilon)$ and $a(x,\varepsilon)$ curves.

The bifurcation diagram for initial boundary value problem (IBVP), which determines the properties of antiphase boundaries (APB) in binary alloys, is considered. It is proven that APBs are asymptotically unstable at all temperatures, but "life time" of such metastable oscillating states may be long. It is well-known that in the case of ordered alloys, typical defects are antiphase domains, which are the results of interaction between atoms of sort *A* and *B* in the binary lattice. In this paper, we study IBVP for a non-conserved order parameter with the classical Neumann (or Dirichlet) boundary conditions. We define the order parameter $u := \rho_A - \rho_B \quad (\rho_A + \rho_B = 1)$ as the difference between the densities of atoms of type *A* and *B*, correspondingly. We show that as $\tau_{\text{int}} \to +\infty$, where τ_{int} is an exchange time between the jumps of atoms *A* and *B* in the lattice, there exist asymptotically stationary oscillating distributions of the order parameter.

There are many problems, where formation of APB in binary alloys is included into consideration, but in previous papers, in typical cases, periodic boundary conditions are considered, and, usually, computer simulations are provided. The results are phase diagrams for special values of parameters of the problem (see, for example, [1]). In this paper, the strong phase (or bifurcation) diagram is constructed, which describes all admissible parameters of the boundary problem. Two situations may arise: the oscillating asymptotic stationary distributions of "spinodal type" may appear, and, for a special type of parameters, when a small parameter ε of the problem exists, there are asymptotically oscillating step-constant distributions.

1. FORMULATION OF THE PROBLEM

Let us consider the thermodynamical potential

$$\frac{F(u)}{k_B T} := \int_0^l \left(f(u) + \frac{1}{2} K(T) |\nabla u|^2 \right) dx, \tag{1}$$

where *f(u)* is the free energy density per unit volume, as given by

$$f(u) := -\frac{1}{2} A(T) u^2 + \frac{1}{4} B(T) u^4, \tag{2}$$

where $A(T)$ changes from negative to positive values at the critical temperature $T=T_g$ for the order-disorder transition; $B(T)$ is positive; $K(T)$ is the positive interfacial energy per unit length; k_B is the Boltzman constant. The temperature T_g is given by the root of equation $A(T) = 0$. Evolution of the order parameter may be described by the Landau-Chalatnikov equation [5]:

$$\frac{\partial u}{\partial t} = -M(T)\frac{\delta F}{\delta u}, \tag{3}$$

where $M(T)$ is the positive reaction rate, $\delta F/\delta u$ is the variational derivative. The equilibrium distributions should be given by

$$\frac{\delta F}{\delta u} := \frac{d}{dx}\left(\frac{dF}{du_x}\right) - \frac{\partial F}{\partial u} = 0. \tag{4}$$

From (4), we obtain

$$G[u] := B(T)\left(\left(u_e(T)\right)^2 - u^2\right)u + M(T)K(T)\nabla^2 u = 0, \tag{5}$$

where $u_e = \left(\frac{A(T)}{B(T)}\right)^{1/2}$. Then equation (3) can be rewritten as

$$\frac{\partial u}{\partial t} = A[u], \tag{6}$$

where $G[u]$ is described by (5). Here, we use the transforms $t \mapsto M(T)t$ and $x \mapsto x/l$.

Further, we consider the Neumann boundary conditions for solutions of (5)

$$u_x(0,t)=0, \quad u_x(l,t)=0, \tag{7}$$

or the Dirichlet boundary conditions

$$u(0,t)=0, \quad u(l,t)=0. \tag{8}$$

From (7), it follows that thermodynamic flux is zero on the walls, which confine binary alloys. According to (8), the binary alloy is in the disordered phase at the walls. Additionally, we consider an initial condition

$$u(x,0) = u_0(x), \quad (0 < x < \pi). \tag{9}$$

If $t\to\infty$, in Sobolev space $H_0^1(0,\pi)$ of distribution [6], the solutions $u(\cdot,t)$ tend to stationary states $\varphi(x), 0 < x< \pi$, which are solutions of equation:

$$\varphi''(x) + a\varphi(x) - b\varphi(x) = 0, \quad 0 < x < \pi, \tag{10}$$

where $a=B(T)u_e(T)^2$ and $b = B(T)$. From [7], it follows that there is a finite number of stationary states in the interval $0 < x < \pi$, i.e. $(2n+1), n=0,1,...,$ if $n^2<a\leq(n+1)^2$ (correspondingly, the transform $n \mapsto n\pi/l$ takes place in the interval $0<x<l$. If $0<a\leq 1$, zero or trivial solution is globally asymptotically stable. If $a > 1$, this solution is unstable as well as all other solutions, with the exception of two solutions, which we define as

φ_1^+, φ_1^-. These asymptotically stable limit distributions have the property $\varphi_1^- < 0 < \varphi_1^+$ for all $0< x < \pi$. A region of attraction of $\{\varphi_1^-, \varphi_1^+\}$ is open dense set in $H_0^1(0,\pi)$.

It is well-known that there is a neighborhood of zero, in $H_0^1(0,\pi)$, that is positive-invariant for all small enough $|a - 1|$. This region is separated in two open sets by stable manifold of the zero solution for small $a - 1 > 0$. We call this two sets by the attractive regions of $\{\varphi_1^-, \varphi_1^+\}$ (see Fig.1, [6]). If B is a sufficiently large ball with the center in the zero in $H_0^1(0,\pi)$, and $u(t, B)$ is the set of all points that are reached by solutions u at the moment of time t, then

$$K = \bigcap_{t\geq 0} u(t, B) \tag{11}$$

is the maximal invariant set. This set is of finite dimension, compact and connected. The set is a union of unstable manifolds of equilibrium states. We have phase portraits that may be found in [6], Fig. 2.

If $n^2 < a \leq (n+1)^2$, the set K has the number of dimensions n, that is a closer of an unstable manifold of zero.

2. THE CHAFEE-INFANTE INITIAL BOUNDARY VALUE PROBLEM

In [7], the following boundary problem is considered:

$$u_t(x,t) = u_{xx}(x,t) + \lambda f(u(x,t)), \quad (0 \leq x \leq \pi,\ 0 < t < +\infty), \tag{12}$$

$$u(0,t)=u(\pi,t)=0, \quad (0<t<+\infty), \tag{13}$$

$$u(x,0)=\varphi(x), \quad (0\leq x\leq\pi). \tag{14}$$

What is the asymptotic solutions of this problem as $t\to+\infty$? The basic tool to solve this problem is the maximum principle for parabolic partial differential equations. Here, $f : R \mapsto R$ is a given continuous function; $\phi : [0,\pi] \mapsto R$ and $\phi \in C^1$ such that $\phi(0) = \phi(\pi)$.

2.1 The Chafee-Infante boundary problem for binary solid solutions

In (12), we may define a function $f(u)$ to be proportional to the function $E'[u]/k_BT$. The parameter λ may be defined as E_{mix}/k_BT, where E_{mix} is so-called mixing energy, and λ describes potential energy (normalized on heat energy) of interaction of atom in the central lattice point with all atoms of the first coordinating sphere, which is equal to $Z(P_{AA}\Phi_{AA}+P_{BB}\Phi_{BB}+2P_{AB}\Phi_{AB})$. The potential energy of the lattice is

$$E := \frac{NZ}{2}\left(P_{AA}\Phi_{AA} + P_{BB}\Phi_{BB} + 2P_{AB}\Phi_{AB}\right), \tag{15}$$

where Z is the coordination number; $N=N_A+N_B$, N_A, N_B are numbers of atoms of sort A, B, correspondingly; P_{AA}, P_{BB}, P_{AB} describe ordering in equilibrium systems. Further, Φ_{AA}, Φ_{BB}, and Φ_{AB} are potential energies of pair interactions of two atoms, which are placed on the distance of radius of the first coordination sphere. Here, the first index describes the type of atom placed in the considered lattice point, and the second index denotes the type of atom on the first coordination sphere. If the lattice is stable, we obtain $\Phi_{AA}<0$, $\Phi_{BB}<0$, $\Phi_{AB}<0$, and $\Phi_{AB}=\Phi_{BA}$, so that in disordered solid solution, we have $P_A=c_A$, $P_B=c_B$, where c_A, c_B are the corresponding concentrations of atoms. Then we can obtain that

$$P_{AB}=c_Ac_B\left(1-2c_Ac_B\left(\exp\left(-E_{mix}/k_BT\right)-1\right)\right), \tag{16}$$

$$P_{AA}=c_A^2\left(1+2c_B^2\left(\exp\left(-E_{mix}/k_BT\right)-1\right)\right). \tag{17}$$

Further, there is a formula [8]: $\Delta\varepsilon_{AB}=-ZP_{AB}E_{mix}$, where $\Delta\varepsilon_{AB}$ is the internal energy released when a solid solution is formed. It is well-known that [8]

$$E:=\frac{NZ}{2}\left(c_A^2\Phi_{AA}+c_B^2\Phi_{BB}+2P_{AB}\Phi_{AB}\right). \tag{18}$$

From (16), it follows that

$$\varepsilon_{AB}=\frac{Z}{2}\left(c_A^2\Phi_{AA}+c_B^2\Phi_{BB}-2P_{AB}\left(c_A,c_B,E_{mix}\right)\right), \tag{19}$$

where P_{AB} is determined by (16).

Without loss of generality, it can be assumed that $E_{mix}/k_BT\ll 1$, where k_BT is of order of heat energy. Then from (16),(17), we obtain that

$$P_{AB}=c_Ac_B\left(1+2c_Ac_B\left(\frac{E_{mix}}{k_BT}-1\right)\right), \tag{20}$$

$$P_{AA}=c_A{}^2\left(1-2c_B{}^2\left(\frac{E_{mix}}{k_BT}-1\right)\right). \tag{21}$$

Thus E_{mix}/k_BT describes the correlation between neighbors atoms, i.e., the short order. For given E_{mix}, with increasing of the temperature, the corresponding correlations are reduced. It will be proved that the value $\chi=E_{mix}/k_BT$, which characterizes intercalation energy, is the bifurcation parameter. This means that solution of the boundary problem, which models an evolution of the order parameter in confined binary alloys, tends to stationary oscillating limit solutions, as time $t\to\infty$. A number of oscillation per interval $0<X<l$ depends on the parameter χ.

If $E_{mix}\neq 0$, but $\chi<<1$, we may use the approximation of ideal solid solution, supposing that $\Delta\varepsilon/k_BT$ is sufficiently small. In this case, $\Delta\varepsilon/k_BT \propto \pm c_A\left(1-c_A\right)$, and we must use the sign (+), if $E_{mix}>0$, and sign(−), if $E_{mix}<0$. Further, we obtain that

$$E=\frac{NZ}{2}\left(c_A^2\Phi_{AA}+c_B^2\Phi_{BB}-2P_{AB}E_{mix}\right), \tag{22}$$

where

$$P_{AB}=c_Ac_B+\frac{2E_{mix}}{k_BT}. \tag{23}$$

Let us suppose $u=c_A-c_B$, where $c_A+c_B=1$. Then from (22), we have

$$E=\frac{NZ}{2}\left(\left|u+c_B\right|^2\Phi_{AA}+\left|u+c_A\right|^2\Phi_{BB}-4E_{mix}\left|u+c_B\right|^2\left|u+c_A\right|^2\frac{E_{mix}}{k_BT}\right). \tag{24}$$

Below we consider perturbations of a nonconserved order parameter at a neighborhood of the disordered phase $u=0$, where $c_A=C_B$. It follows from the last equality that we can use $c_A\simeq c_B\simeq 1/2$, where 1/2 plays the role of probability. Now we define $u\mapsto u+1/2$, and rewrite (24) in the form

$$\frac{E[u]}{k_BT}=\frac{NZ}{2}\left(A|u|^2+B|u|^2-4|u|^4\left(\frac{E_{mix}}{k_BT}\right)^2\right), \tag{25}$$

where $A=\Phi_{AA}/k_BT$, and $B=\Phi_{BB}/k_BT$. Then

$$\frac{E'[u]}{k_BT}=NZ\left(A+B\right)u-6NZ\chi^2u^3. \tag{26}$$

The linear approximation at the point $u = 1/2$ results in the determination of energy:

$$\frac{E[u]}{k_BT}=\frac{1}{2}NZ\left(A+B\right)-\left(\frac{3}{4}NZ\chi^2+NZ\left(A+B\right)-\frac{9}{4}NZ\right)\chi^2\left(u-\frac{1}{2}\right)+O\left(u-\frac{1}{2}\right). \tag{27}$$

Transforming $u\mapsto u-1/2$, from (27), we obtain for the derivative

$$\frac{E'[u]}{k_BT}=\frac{1}{2}NZ\left(A+B\right)-\lambda u+O\left(u\right) \tag{28}$$

at the point $u = 0$, where $\lambda:=\left(\frac{3}{4}NZ\chi^2+NZ\left(A+B\right)-\frac{9}{4}NZ\right)\chi^2$ and $\kappa:=\frac{1}{2}NZ\left(A+B\right)$. Let us establish $u\mapsto u+\frac{\kappa}{\lambda}$. Then from (28), we obtain that

$$\frac{E'[u]}{k_BT}=-\lambda u+O\left(u\right) \tag{29}$$

at disordered phase.

Further, for a disordered solid solution, entropy S_{AB} can be represented in the form [8]:

$$S_{AB} = S_{id} + S_{mix}, \tag{30}$$

where S_{id} is the entropy of an ideal solid solution, and S_{mix} is the entropy of mixing. It is well known that for ideal solid solutions, the second term in (30) can be neglected. The first term is

$$\frac{S(c_A, c_B)}{k_B T} = \frac{c_A}{N_A}\ln c_A + \frac{c_B}{N_B}\ln c_B, \tag{31}$$

where $N_A+N_B=N$. Assuming that $c_A=c_B=c$, we obtain the curve of phase coexistence:

$$\frac{1}{N}\ln\left(\frac{c}{1-c}\right) + \lambda(1-2c) = 0. \tag{32}$$

3. THE ALLEN-CAHN EQUATION

Further, we consider the Allen-Cahn equation, which represents a gradient flow for the free energy functional

$$\mathcal{E}[u] = \int_0^1 \left(\frac{1}{2}|u_x|^2 - F'(u)\right)dx, \tag{33}$$

where $F'(u) = f(u)$ and $0 < x < l$ is the spatial domain, which is occupied by the binary alloys under consideration. Here,

$$f(u) = \lambda u + \ln\left(\frac{u}{1-u}\right), \tag{34}$$

where the first term follows from the linear approximation of ordering energy for an ideal solid solution. The second term, at $u = 1/2$, is

$$\ln\left(\frac{u}{1-u}\right) = -\frac{1}{N}u + O\left(u-\frac{1}{2}\right). \tag{35}$$

Hence, $-F'(u) = \lambda - \frac{1}{N}$. We consider the case $\lambda > 1/N$ when there is phase decomposition of disordered phase on two ordered phases. Further, $\kappa \sim U r_0^2$, where U is the interface energy between ordered and disordered phases; r_0 is the correlation radius between atoms of solid solution.

A corresponding gradient flow is [3-5]:

$$u_t = -\gamma(u)\frac{\delta\mathcal{E}}{\delta u}, \tag{36}$$

where $\delta\mathcal{E}/\delta u$ is the $\mathcal{L}^2$ functional derivative of $\mathcal{E}$. The result is

$$u_t = \gamma(u)\left[\kappa(u)u_{xx} - \frac{1}{2}\kappa'(u)u_x\Big|^2 - f(u)\right]. \quad (37)$$

The linear version (at $u = 0$, that is, at disordered phase) is

$$u_t = Du_{xx} + au - bu^3, \quad (38)$$

where we use the representation (26) for $f(u)$, so that $a = NZ(A+B)u$ and $b=6NZ\chi^2u^3$ ($\chi=\lambda-1/N$). In the general case, $A + B \propto \left(1 - T/T_g\right)$, where T_g is the critical temperature of decomposition of a homogeneous disordered binary solid solution (see [5]). Here, $t \mapsto \gamma t$, $D = \kappa(0)$ where $\kappa(0) = \frac{U}{k_B T}\left(\frac{r_0}{l}\right)^2$.

Then, applying formal results of [7], we obtain following statements: If $t\to+\infty$, solutions $u(\cdot,t)$ tends to a stationary state φ in the Sobolev space $H_0^1(0,\pi)$ that is a solution of the problem [6]:

$$\varphi_{xx} + \tilde{a}\varphi(x) - \tilde{b}\varphi^3(x) = 0, \quad (39)$$

where $\tilde{a}=NZ(A+B)/D$ and $\tilde{b} = 6NZ\chi^2u^3/D$. It follows from (39) that

$$u_t = \varphi_{xx} + \lambda\left(\varphi_e - \varphi^2\right)\varphi = 0, \quad (40)$$

where $\lambda=b$ and $\varphi_e = \tilde{a}/\tilde{b}$.

The Dirichlet boundary conditions are

$$\varphi(0) = 0, \quad \varphi(l) = 0. \quad (41)$$

Chafee and Infante [7] proved that, if $n^2 < a <\leq (n+1)^2$, $n = 0,1,2,...$, there are $(2n+1)$ stationary points $\varphi_0 = 0$, and $\varphi_k^{\pm}$ $(k = 1,...,n)$, where $(d/dx)\varphi_k^+ > 0$ at $x = 0$, as $n^2<a<\leq(n+1)^2$, $(d/dx)\varphi_k^- < 0$ at $x = 0$, and the function $\varphi_k^{\pm}$ has $(k-1)$ zeros on interval $0 < x < \pi$. Further, if $\lambda > 1$, $\varphi_k^{\pm}$ are asymptotically stable in linear approximation, but φ_0 and $\varphi_k^{\pm}$ $(2 \le k \le n)$ are together asymptotically unstable.

4. SPIKE-TYPE ASYMPTOTICALLY STATIONARY STABLE STRUCTURES IN CONFINED BINARY MIXTURES

The results of [9] show that periodic APBs have two competing annealing processes: the annihilation of APBs trough formation of peak stationary distributions (Fig.1). This distribution appears as parameter $\varepsilon=K(T)/l^2$ becomes small, whereas $K(T)$ plays the role of "mobility". Indeed, let us study the boundary-value problem

$$u_t=M(T)K(T)u_{xx}+M(T)B(T)(u_e(T)^2-u^2)u. \quad (42)$$

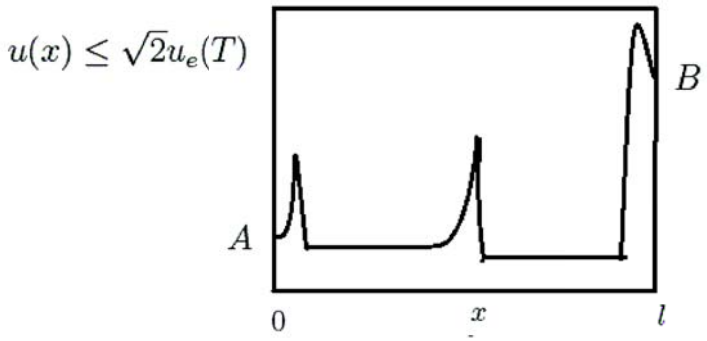

Fig. 1. Peak stationary distributions of the nonconsereved order parameter in a binary alloy.

Let us assume $t \mapsto M\left(T\right)/l^2$, and $x \mapsto x/l$. Then, from (42), we obtain that

$$u_t = \epsilon u_{xx} + B(T)\left(u_e\left(T\right)^2 - u^2\right)u \equiv h\left(u\right), \tag{43}$$

where ε=$M(T)/l^2$. We suppose εll1, and consider the Dirichlet boundary condition

$$u(0,\varepsilon)=\tilde{A}, \quad u(1,\varepsilon)=\tilde{B}, \tag{44}$$

which means that surface atoms are in "partially ordered" phase. This fact may be interpreted as surface segregation of atoms with surface densities $\rho_A\left(0,t\right)-\rho_A\left(B,t\right)=0$ and $\rho_A\left(1s,t\right)-\rho_A\left(B,1\right)=B$, where A,B are constants. In literature, only the case of A=B=0 is considered, where the surface atoms are in the disordered state.

4.1. The degenerated case

At ε = 0, the degenerated equation (42), or $h(y)$=0, has three stationary solutions $u_{1,3}\left(x\right)\equiv\pm u_e\left(T\right)$ and $u_2(x)$≡0. Since $h'(u_2)$>0, $h'(u_1)$=$h'(u_3)$<0, only the solution u=$u_2(x)$ is stable.

Using the integral condition of stability [10] for solutions of boundary problem (42),(44), which has the form

$$\int_0^{\varsigma} B\left(T\right)\left(u_e\left(T\right)^2 - s^2\right)sds > 0 \tag{45}$$

(see also, [5] and [10], p.53). Simple calculations of integral result in the inequality $\left|\varsigma\right| < \sqrt{2}\left|u_e\left(T\right)\right|$. Hence, from the result of O'Mally [10], the statement follows: if $\left|\tilde{A}\right|, \left|\tilde{B}\right| < \sqrt{2}\left|u_e\left(T\right)\right|$; then there are solutions where the limit relation

$$\lim_{\varepsilon\to+\infty} u\left(x,\varepsilon\right)=0, \quad x\in\left[\delta,1-\delta\right] \tag{46}$$

is valid.

In addition to solutions (46) of boundary-layer type, as ε→→0, the considered boundary problem has oscillating solutions of the peak-type layer when a solution tends,

to zero for all points on interval [0,1] as ε→→0, with exception of some number of points of the interval, which are placed at equal distance from one to another (see Fig. 1). In some neighborhood of every point, for sufficiently small ε>0, this solution has a narrow peak. This peak does not tend to zero as ε→0.

This result follows from [10], at the point $u_2(x)\equiv$ the integral

$$\Psi[u]=\int_A^u B(T)\left(u_e(T)^2-s^2\right)sds \tag{47}$$

has the maximal value, i.e. the potential energy of the system is maximal. We have also $\Psi\left[u=\sqrt{2}\left|u_e(T)\right|\right]=\Psi[0]=0$, if $|A|<\sqrt{2}\left|u_e(T)\right|$, and the value $u=\sqrt{2}\left|u_e(T)\right|$ is not the point of maximum of function Ψ[*u*]. This result means that, for any integer $n\geq 0$, the boundary problem has four solutions $u=u(x,\varepsilon)$, if $|A|<\sqrt{2}\left|u_e(T)\right|$ and $|B|<\sqrt{2}\left|u_e(T)\right|$, satisfying the limiting relation

$$\lim_{\varepsilon\to+\infty} u(x,\varepsilon)=0,\quad x\in[\delta,1-\delta] \tag{48}$$

with $\delta\in(0,1/2)$, except the points $x_i=i/n,\quad i=\overline{1,n-1}$, where the limit relation is satisfied:

$$\lim_{\varepsilon\to+\infty} u(x,\varepsilon)=\pm\sqrt{2}\left|u_e(T)\right|. \tag{49}$$

For $n=2$, we have one peak, and for $n=3$ we have two peaks. In the general case, amplitudes may not be equal (see, for example, Fig. 1).

4. THE CONTRAST STRUCTURES

Now we consider the bistable Cahn-Hilliard equation [3, 11]

$$u_t=M^-(T)\left(K^-(T)u_{xx}-f(u)\right),\qquad 0<x<l, \tag{50}$$

where the diffusion coefficient $K^-(T)/l^2$ is small. The parameter $M^-(T)/\tau_{diff}=O$ is large, so that $K^-(T)M^-(T)=O(1)$, where $O(1)$ is a bounded value; τ_{diff} is the typical time of diffusion of atoms. As shown in [3], we obtain from this condition that there are solutions in the form of internal layers of thickness $O(k^{-1/2})$. The layers move with the phase velocity

$$V=-M^-(T)K^-(T)R, \tag{51}$$

where *R* is the mean curvature of a layer.

We rescale the time variable *t*, so that $t\mapsto t/\epsilon^2$, where $t\mapsto M^-(T)$; and we transform the spatial variable *x*, so that $x\mapsto x/\epsilon^2$, where $x\mapsto x/l$. Then equation (50) can be rewritten as

$$\epsilon^2 u_t = \epsilon^2 K^-(T) u_{xx} + B(T)\left(u_e(T)^2 - u^2\right)\left(u - a(x,\epsilon)\right), \quad 0 < x < l. \qquad (52)$$

Further, we introduce new time variable $t \mapsto K^-(T)t$ and rewrite (52) as

$$\epsilon^2 u_t = \epsilon^2 u_{xx} + \left(B(T)/K^-(T)\right)\left(u_e(T)^2 - u^2\right)\left(u - a(x,\epsilon)\right), \quad 0 < x < l. \qquad (53)$$

Here, we introduce the function $a(x,\epsilon)$, which describes the spatial-temporal inhomogeneities in the disordered phase. As $\epsilon = 0$, there are two stationary solutions $u(x,t) = \pm u_e(T)$. The points $\pm u_e(T)$ correspond to two minimums of the free energy. Further, let us introduce the point $a(x,\epsilon)$, which corresponds to the maximum of free energy. This point determines a boundary between the areas of influence of the left stable zone $u=-u_e(T)$ and the right one $u=u_e(T)$.

It is well-known (see, for example, [2,12]) that equation (52) with the homogeneous Neumann boundary condition and with the initial state $u(x,0) = u_0(x)$, has asymptotically stable solutions presented in Fig.2. The phase boundary is established as the intersection point between the graphics of functions $a(x,\epsilon)$ and $u_0(x)$. It is evidently, how this boundary changes, if $a(x,\epsilon) \equiv 0$. Thus we obtained the distributions of APB that may be called contrast structures [2, 12].

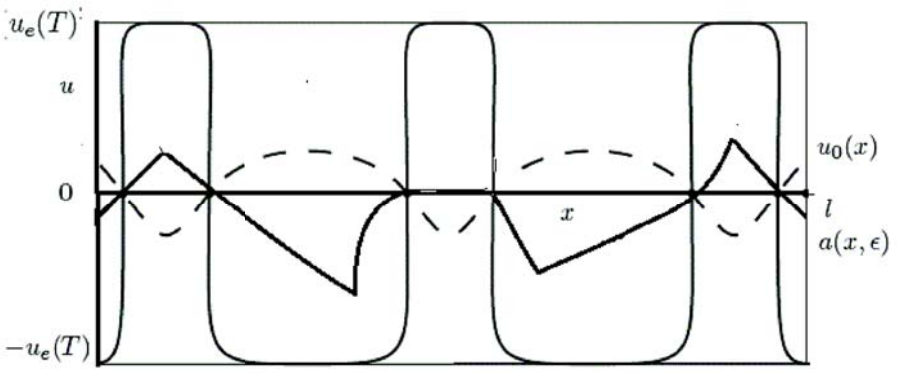

Fig. 2. Contrast asymptotically stationary structures in binary alloys.

CONCLUSIONS

We investigated the dynamics of formation of asymptotic stationary domains at isothermal ageing in binary alloys. This dynamics may be observed by a microscop as a dark field image (see [1]). The first considered case is the evolution of APBs, or antiphase ordered domains, in an alloy with so-called contrast structures, which are step-constant oscillating stationary structures described by the nonconserved order parameter with

Neumann's boundary conditions. These structures, as shown in [1], are observed in substitution binary alloys. The obtained theoretical results are compared with the scenario of formation of APBs in Fe_3Al at ordering $B2$ to DO_3. The second case is the classical APD of sinusoidal type. The third case is the phase separation, which results in formation of so-called peak-type structures that can be reduced, if the dimensionless diffusion of atoms is small. The APBs of sinusoidal type have been observed for small oscillations of the order parameter at the disordered phase. But the contrast structures and peak-type structures are obtained for finite amplitudes of order parameters.

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Краснюк И. Б. Эволюция антифазных упорядоченных доменных структур в ограниченных бинарных сплавах / Краснюк И. Б., Мельник Т. Н., Юрченко В. М. // Ученые записки Таврического национального университета имени В.И. Вернадского. Серия: Физико-математические науки. – 2012. – Т. 25(64), № 1. – С. 193-205.

Рассмотрена начально-краевая задача с граничными условиями Дирихле и Неймана. Эта задача описывает эволюцию несохраняющегося параметра порядка в бинарных сплавах вблизи неупорядоченной фазы. Показано, что задача имеет асимптотически осциллирующие стационарные распределения параметра порядка. Эта осцилляция описывает так называемые антифазные границы (АФГ) в бинарных сплавах. Построена соответствующая фазовая диаграмма. В частности, показано, что температура является бифуркационным параметром, поэтому при охлаждении в ограниченных бинарных сплавах на больших временах появляются стационарные антифазные границы с различным числом осцилляций между стенками, ограничивающими образец. Далее показано, что если в системе

имеется малый параметр, то наличествуют и контрастные структуры – ступенчатые асимптотически стационарные распределения АФГ.
Ключевые слова: бинарныесплавы, антифазные границы.

Краснюк І. Б. Еволюція антифазних впорядкованих доменних структур в обмежених бінарних сплавах / Краснюк І. Б., Мельник Т. М., Юрченко В. М. // Вчені записки Таврійського національного університету імені В.І. Вернадського. Серія: Фізико-математичні науки. – 2012. – Т. 25(64), № 1. – С. 193-205.
Розглянуто початково-крайову задачу з граничними умовами Діріхле та Неймана, яка описує еволюцію параметру порядку, що не зберігається, в бінарних сплавах поблизу невпорядкованої фази. Показано, що задача має асимптотично осцилюючі стаціонарні розподілення параметру порядку. Ця осциляція описує так звані антифазні межі (АФМ) в бінарних сплавах. Побудовано відповідну бифуркаційну діаграму. Зокрема, показано, що температура є бифуркаційним параметром, тому під час охолодження в обмежених бінарних сплавах за великого часу з’являються стаціонарні антифазні межі з різним числом осциляцій між стінками.. Далі показано, що якщо в системі є малий параметр, то є присутніми і контрастні структури – асимптотично кусочно-постійні стаціонарні розподілення АФМ.
Ключові слова: бінарні сплави, антифазні межі.

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