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Research article

Dynamic boundary conditions in the interface modeling of binary alloys

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Abstract: We study the initial boundary value problem with dynamic boundary conditions to the Penrose-Fife equations with a 'memory effect' for the order parameter and temperature time evolutions. The dynamic boundary conditions describe the process of production and degradation of surface crystallite near the walls, which confine the disordered binary alloy at a nearly melt temperature during the fast cooling process. The solid-liquid periodic distributions, which were obtained in $1D$ case, represent asymptotically periodic piecewise constant spatial-temporal impulses in a long time dynamics. It is confirmed that, depending on parameter values, the total number of discontinuity points of such periodic impulses can be finite or infinite. We refer to such wave solution types as relaxation or pre-turbulent, respectively. These results are compared with experimental data.

Keywords: phase-field equations; difference equations; pre-turbulent; turbulent; global attractor
Mathematics Subject Classification: 35B10, 34B60

1. Introduction

This paper is a continuation of the previously published results [12], where the authors studied a boundary value problem for a system of Allen-Cahn, Cahn-Hilliard and heat transfer (with account of latent heat) equations with no-flux boundary conditions. This system models distributions of a conserved order parameter (u), non-conserved one (v) and temperature (θ). It was shown that there exists a solution of the problem which consists of long-time oscillating functions. Such solutions describe experimentally observed fluctuations of the order parameter, concentration and temperature in confined binary alloys or binary polymer mixtures. In the present paper, we consider the following system:

$$\tau_u u_{tt} + u_t = [\omega_1 Q(u,v)(F'_u(u,v,\theta) - \varepsilon^2 u_{xx})_x]_x, \tag{1}$$

$$\tau_v v_{tt} + v_t - \sigma\tau_v\theta_t = \omega_2 Q(u,v)(\varepsilon^2 v_{xx} - F'_v(u,v,\theta)) + \sigma\theta, \tag{2}$$

$$\tau_\theta \theta_{tt} + \lambda \tau_\theta v_{tt} + \theta_t + \lambda v_t = D\theta_{xx} \tag{3}$$

with the dynamic boundary conditions:

$$u_t(k,t) = N_k[u(k,t)],\ v_t(k,t) = G_k[v(k,t)],\ \theta_t(k,t) = \Upsilon_k[\theta(k,t)],\ k = 0, l. \tag{4}$$

All parameters for the problem (1)–(4) will be given later in Section 2. We will refer to (1) as modified Cahn-Hilliard equation and to (2), (3) as modified Penrose-Fife equations.

Unlike the conditions assumed for the model studied in [12], in the present paper we take into account 'memory effects' for fluxes and we also implement dynamic boundary conditions to capture a feedback effect. As noted in [21], "Feedback processes are fundamental in all exact sciences. In fact, they were first introduced by Sir Isaac Newton and Gottfried W. Leibniz some 300 years ago in the form of dynamic laws". It turns out that a general melting process exhibits 'surface' order-disorder transition, so that wave perturbations with feedback become dominant in the organization of bulk structures of waves. In this sense, one can talk about surface-induced structures of relaxation, pre-turbulent, or turbulent types in real physical systems with the surface feedbacks. The feedback machine consists of the following components: input, output, control unit, processing unit, and one main processor, which are all connected by four transmission lines (see [21, Figure 1.3]). One-step machine algorithms can be characterized by the iterations $u(t+1) = f[u(t)]$, where $f : I \to I$ is a non-linear function and I is some bounded interval. For example, we can consider a well-known logistic map $f : u \to au(1-u)$, where $a \in [0,4]$ is the bifurcation parameter, and $I := [0,1]$. In our situation, we propose to control behaviour of solution near the boundary by the dynamic boundary conditions, i. e. by using a special choice of inputs and outputs. From experimental point of view, the dynamic boundary conditions describe a process in an alloy near the surface where bubbles propagate into a bulk. These surface bubbles penetrate into the bulk along trajectories which are close to characteristics of correspondent linear hyperbolic equations. Using dynamic boundary conditions, we can reduce our original PDE problem to a system of difference equations. In some particular cases, asymptotic properties of solutions for this system can be deduced from iterations of a one-dimensional map (for example, quadratic or logistic).

The evolution process of the conserved order parameter u will be described by the modified Cahn-Hilliard (*mCH*) equation that was originally introduced by Galenko et al. [16]. This equation models the non-Fickian diffusion of the binary alloys in so-called tau-approximation, which describes the 'memory' of the alloy. Then the *mCH* equation follows from the relation

$$\tau_u J_t(\cdot,t) + J(\cdot,t) = -M(u,\theta)(F'_u(u,u_x) - \varepsilon_u^2 u_{xx})_x \tag{5}$$

with the non-Fickian diffusion flux J, and $\theta = 1 - T/T_m$, where T_m is the melt temperature of crystallization on front of liquid phase at a neighbourhood of the disordered state, u is one component of a binary alloy. Here, $F := F(u,u_x)$ is the free energy, $\varepsilon_u^2 = 2F_0\xi_b^2$, F_0 is the dimensionless energy of interaction between atoms of A and B types, ξ_b is the characteristic length, M is the mobility of atoms, and τ_u is the relaxation time. The *mCH* equation has simple physical meaning. Namely, if the front velocity for crystalline phase is small enough then the evolution of wetting phase is described by the classical Cahn-Hilliard (*CH*) equation. If this velocity is large enough then the crystalline phase is described by the *mCH* equation because the non-Fickian flow corresponds to a change of the front velocity due to a time delay. In the last case, we have to replace the *CH* equation with the *mCH* equation. In [16], it is shown that the decomposition in binary systems can be described by the *mCH* equation in the following cases: (a) local in time dynamics; (b) large characteristic velocities; (c) large gradients of the concentration; (d) deep super-cooling.

Note that unlike the modified Cahn-Hilliard equation the Penrose-Fife type equations are very difficult to solve by using Onsager thermodynamic formalism, because one have to deal with the non-conserved order parameter and temperature which are coupled by time derivatives, and as a result, the problem does not allow a variational formulation. According to [7, Eq. (73),(74), p.113]), the system of Penrose-Fife equations is written as:

$$\gamma\epsilon^2\phi_t = \epsilon^2(1 + \tau(T - T_m))\phi_{xx} - F'_\phi - \alpha\beta^2\epsilon^2 T\phi_x(1/T)_x, \tag{6}$$

$$e_t = (KT_x)_x + \beta^2\epsilon^2[\phi_t\phi_{xx} - \alpha(\phi_x\phi_t)_x]. \tag{7}$$

where ϕ is order parameter, e is internal energy, T is temperature, T_m is a melting temperature, K is the thermal conductivity, $F = F(T, \phi)$ is the local density of the Helmholtz free energy, $\beta^2 = 1 - \tau T_m$, γ is the basic order parameter kinetic coefficient, τ and ϵ are some dimensionless parameters. These equations are reduced to the well-known model A if $\alpha = 0$, and to the model B if $\alpha = 1$. The A, B models are both of Ginsburg-Landau type and hence, are examples of phenomenological models. If we assume that K is constant, $e = T + \lambda\varphi, \beta = 0$ and $T \approx T_m$, then equations (6), (7) can be reduced to

$$\gamma\epsilon^2\phi_t = \epsilon^2\phi_{xx} - f'_\phi(T, \phi), \tag{8}$$

$$T_t + \lambda\phi_t = K\,T_{xx}. \tag{9}$$

Therefore, the system (8)–(9) corresponds to the modified Penrose-Fife equations (2)–(3) with $v = \phi$, $\theta = T$, $\tau_v = \tau_\theta = 0$, with Q and F linearised about $(u, v, \theta) = (1/2, 0, 0)$. Also, the modified Cahn-Hilliard equation and the modified Penrose-Fife equations describe the non-Fickian processes (see Section 2).

In [12, 15] we have studied a boundary value problem for a system of Allen-Cahn, Cahn-Hilliard and heat transfer equations with Neumann boundary conditions. It was shown that there exists a family of solutions with long-time oscillations. Stationary oscillations for the concentration and the order parameter were known in binary alloy theory but stationary oscillations for the temperature was a new result. What happens with long-time oscillations if instead of the Neumann boundary conditions, one implement non-linear dynamic boundary conditions? In this case we obtain spatial-temporal limit distributions of concentration, order parameter and temperature, depending on the travelling wave variable $s = t - x/V$, where V is the velocity of propagation. It should be mentioned that this result is still holds true if instead of the classical Penrose-Fife equations (see [6, 22]) we consider the modified hyperbolic Penrose-Fife equations.

The main idea of deriving modified equations is the following one: consider a general continuity equation for some quantity u:

$$u_t = -J_x + f, \tag{10}$$

where J is a flux, f is the mass force. According to the Fourier's law (or Fick's law), we know that

$$J = -Du_x, \tag{11}$$

where D is the diffusion coefficient. If D is a constant then by (10), (11) we arrive to the classical heat equation:

$$u_t = Du_{xx} + f. \tag{12}$$

It is well-known that (12) has infinite speed of support propagation for perturbations but this definitely contradicts experimental results. There are many ways how to approach this paradox. One of possibilities is to take into account inertia effects of the flux. This method leads to the following non-Fickian law:

$$J(t + \tau) = -Du_x,$$

where τ is some relaxation time. For example, for the most of different types of metals the thermal relaxation time is of the order of picoseconds. Approximating $J(t + \tau) \approx J(t) + \tau J_t(t)$, we get the Maxwell-Cattaneo law:

$$J(t) + \tau J_t(t) = -Du_x. \tag{13}$$

Differentiating (10) with respect to t and (13) with respect to x, we obtain

$$u_{tt} = -J_{xt} + f_t', \quad J_x + \tau J_{xt} = -Du_{xx},$$

whence

$$\tau u_{tt} = Du_{xx} + J_x + \tau f_t'.$$

From here, due to (10), we obtain the following telegraph equation

$$\tau u_{tt} + u_t = Du_{xx} + g, \tag{14}$$

where $g = f + \tau f_t'$. It is well-known that (14) has finite speed of support propagation for perturbations. Hence, the paradox is finally resolved. Obviously, (14) coincides with (12) if $\tau = 0$. Following this way in Section 2, we derive a system (1)–(3).

In the present paper, we show that the process of crystallisation of a melt can be described by the coupled modified Cahn-Hilliard (CH) and Penrose-Fife (PF) equations which describe the alloy's dynamic in a neighbourhood of the equilibrium point $a = (u, v, \theta) = (1/2, 0, 1 - T_0/T_m)$, where T_m is a melting temperature. At the point a this system splits into a linear CH equation and two coupled linear PF equations. In this case the original problem is getting reduced to the study of PF equations only, that describe a process of ordering of atoms' types A and B which are initially in the disordered state which normalized by $A + B = 1$. Then, after cooling of the alloy on the flat walls, the front of crystallization arises at the boundary of a pattern and propagates into the melt. Next, we assume that this process can be formally described by the dynamic boundary conditions (4).

We are interested in existence of travelling wave type solutions for the linearised system (1)–(3). We use the method of reduction of the boundary value problem to the initial value problem for the system of difference equations with continuous time. These difference equations form hyperbolic dynamical system for which we can to apply the method developed by Sharkovsky (see [29]). By this reduction we show that there exist locally (in a neighborhood of an equilibrium point) oscillating spatia-temporal asymptotic solutions with a finite or an infinite number of discontinuity points on their periods. For example, if one of these boundary functions has at least one internal extremum then wave oscillations of order parameter and temperature arising in the bulk belong to the pre-turbulent type. If one of these functions is monotone on the interval $(0, l)$ with two attractive and one repelling fixed points, then the PF system is bistable. In this case, we obtain asymptotic periodic impulse function with constant amplitudes and the one point of discontinuities on a period (see, Figure 2). Note that these periodic functions are smooth for smooth initial data, excluding the point $t = +\infty$ (see [29]). Note that discontinuities of smooth solutions across the interface arise when $t \to +\infty$. Otherwise, the solutions are smooth at each finite time $t > 0$ under an assumption that initial data of the problem are also smooth. An attractor of the system represents a set of generalized functions (see [29]) which are piecewise constant periodic functions. Solutions can have different sets of discontinuities: finite, infinite, countable or uncountable, and we refer to such solutions as relaxation, pre-turbulent or turbulent type, respectively. We reference a reader to [29, Definition 1.5, p. 154] for details about solutions of relaxation, pre-turbulent and turbulent types. The type of the long time limit of a periodic solution depends on the topological structure of the mapping $\Phi : \mathbb{R}^2 \to \mathbb{R}^2$ which is controlled by the dynamic boundary conditions of the problem. The mapping Φ leads to a system of two difference equations with continuous time. This mapping is hyperbolic, and structurally stable with only a finite number of attractive and repelling points in $\mathbb{R}^2$.

Also, we show that this linearised equations (1)–(3) with non-linear boundary conditions (4) accurately describe the surface-induced spatial-temporal structures of wave type which enter into the bulk as 'solitons'. Limit distributions of the order parameter and temperature are periodic piecewise constant functions with a finite or an infinite number of discontinuity points on a period. The topological form of these functions is determined by the topological form of the boundary conditions. Moreover, these functions are elements of attractors of the corresponding dynamical system. The structure of such an attractor also depends on the initial data. Elements of the attractor can be deterministic or random functions (see [14, 26, 27, 28, 29]). As noted in [8, p.70], "Despite decades of research, the growth of lamellar eutectic in bulk sample is still not well understood". We consider a mathematical model which can be applied to the study of formation and evolution of spatial-temporal lamellar eutectic structures of relaxation, pre-turbulent and turbulent type (see Figure 3). These solutions describe 'one-dimensional' micro-structures with finite, countable or uncountable boundaries, which arise due to the solidification process.

The paper is organized as follows. In Section 2, we formulate the initial boundary value problem for the linear Penrose-Fife equation and the Cahn-Hilliard equation with dynamic boundary conditions and initial data satisfying the smooth fitting conditions at the endpoints $x = 0$ and $x = l$, where l is the size of a sample. We use the observation that these equations at the equilibrium point can be decomposed as the CH equation, which is independent of order parameter and temperature, and as the coupled Penrose-Fife equations. By this reason, we will study the boundary value problem for the PF equations only. In Section 3, it will be shown that the initial boundary value problem can be reduced to the initial value problem for the system of difference equations with continuous time. Moreover, in Sections 3 and 4, we will consider an example when all functions in boundary conditions are linear except one that is in the boundary condition for temperature. In this case, the problem reduces to the quasi-one-dimensional difference equation in $\mathbb{R}^2$, which, respectively, can be analyzed by application of the quadratic map. Additionally, in Section 5 we consider applications to experiments and discuss the physical interpretation of the dynamic boundary conditions.

2. The problem statement

In this section, we linearise the modified Cahn-Hilliard equation, the Penrose-Fife equation and the heat transfer equation about the equilibrium $(u, v, \theta) = (1/2, 0, \theta_0)$, where θ_0 is a critical temperature, and we consider the long-time asymptotic behaviour of solutions. First of all, we derive these modified equations. Hence, let us consider the following system of equations (see [12]):

$$u_t = [\omega_1 Q(u,v)(F'_u(u,v,\theta) - \varepsilon^2 u_{xx})_x]_x, \quad \omega_1 \in \mathbb{R}^+, \tag{15}$$

$$v_t = \omega_2 Q(u,v)(\varepsilon^2 v_{xx} - F'_v(u,v,\theta)) + \sigma\theta, \quad \sigma \in \mathbb{R}, \quad \omega_2 \in \mathbb{R}^+, \tag{16}$$

$$\theta_t + \lambda v_t = D\theta_{xx}, \quad \lambda \in \mathbb{R}, \tag{17}$$

where u is a conserved order parameter, v is a non-conserved order parameter, θ is temperature,

$$Q(u,v) = u(1-u)(1/4 - v^2) \geqslant 0 \tag{18}$$

is mobility, λ is latent heat parameter, ω_1, ω_2 are positive constants (below, we take $\omega_1 = \omega_2 = 16$). These equations represent the simplest form of the phase field model (see [6, 22]). In this case, the Ginzburg-Landau functional can be written as:

$$E = \int_0^l [F(u,v,\theta) + \frac{\varepsilon^2}{2}(u_x^2 + v_x^2)]dx, \tag{19}$$

where

$$F(u,v,\theta) = \frac{\theta}{2}[G(u+v) + G(u-v)] + \chi u(1-u) - \beta v^2 \tag{20}$$

is a free energy, χ and $\beta \in \mathbb{R}$,

$$G(s) = s\ln s + (1-s)\ln(1-s) \tag{21}$$

is entropy. Equations (16)–(17) are Penrose-Fife equations. Next, if we assume that a characteristic relaxation time of the temperature field is much faster than a relaxation time of concentration and that the heat transfer of both phases is described by the parabolic equation. If a characteristic relaxation time for the order parameter is much smaller than the relaxation time for the temperature then we obtain the parabolic equation for the order parameter (the classic Allen-Cahn equation) and the hyperbolic equation for the temperature in the Penrose-Fife system. Note that if it is not true then both Penrose-Fife equations are of hyperbolic type.

Next, assume that all fluxes satisfy the non-Fickian generalised law, i. e.

$$\tau_u J_{1,t} + J_1 + \omega_1 Q(u,v)(F'_u(u,v,\theta) - \varepsilon^2 u_{xx})_x = 0, \tag{22}$$

$$\tau_v J_{2,t} + J_2 + \omega_2 Q(u,v)(\varepsilon^2 v_{xx} - F'_v(u,v,\theta)) = 0, \tag{23}$$

$$\tau_\theta J_{3,t} + J_3 + D\theta_x = 0, \tag{24}$$

where τ_u, τ_v, τ_θ are the corresponding relaxation times. Using the following relations

$$u_t = -J_{1,x}, \; v_t = -J_2 + \sigma\theta, \; \theta_t + \lambda v_t = -J_{3,x},$$

by (22)–(24) we arrive at

$$\tau_u u_{tt} + u_t = [\omega_1 Q(u,v)(F'_u(u,v,\theta) - \varepsilon^2 u_{xx})_x]_x, \tag{25}$$

$$\tau_v v_{tt} + v_t - \sigma\tau_v\theta_t = \omega_2 Q(u,v)(\varepsilon^2 v_{xx} - F'_v(u,v,\theta)) + \sigma\theta, \tag{26}$$

$$\tau_\theta\theta_{tt} + \lambda\tau_\theta v_{tt} + \theta_t + \lambda v_t = D\theta_{xx}. \tag{27}$$

Note that the system (25)–(27) coincides with (15)–(17) when $\tau_u = \tau_v = \tau_\theta = 0$. This approach was used in the study of the Cahn-Hilliard equation with delay argument for application to polymer blends with dynamic boundary conditions in [11, 14]. These equations describe evolution of distributions with non-Fickian diffusion and represent 'tau-approximation' for 'numerical turbulence'. Moreover, this idea was also used by James Clerk Maxwell for heat transfer equation (see [3, 19]). Next, linearising (25)–(27) about the equilibrium point $(u, v, \theta) = (1/2, 0, 0)$, we obtain the following system of equations

$$\tau_u u_{tt} + u_t = -\varepsilon^2 u_{xxxx} - 2\chi u_{xx}, \tag{28}$$

$$\tau_v v_{tt} + v_t - \sigma\tau_v\theta_t = \varepsilon^2 v_{xx} + 2\beta v + \sigma\theta, \tag{29}$$

$$\tau_\theta\theta_{tt} + \lambda\tau_\theta v_t + \theta_t + \lambda v_t = D\theta_{xx}. \tag{30}$$

As a result, the linearised Cahn-Hilliard and Penrose-Fife equations are uncoupled, and we can consider the Penrose-Fife equations separately by using the following dynamic boundary conditions (4), where N_k, G_k, $\Upsilon_k : I \to I$; $k = 0, 1$ are the given smooth functions, $I := [0, l]$ and $\theta = 1 - T/T_m$. Note that the boundary conditions describe 'probability' density of crystallite injection with feedback into the bulk after cooling below $T < T_m$. We conclude that, for special initial conditions of exponential type, the attractor of the Penrose-Fife problem contains piecewise constant periodic functions $p_1(s)$, $p_2(s)$ (see Figure 2), where $s = t - x/V$.

3. Travelling wave solutions to the initial boundary value problem

Using that the Cahn-Hilliard equation (28) is uncoupled from the system (29), (30) we can study separately the linearised hyperbolic Penrose-Fife equations:

$$\tau_v v_{tt} + v_t - \sigma\tau_v\theta_t = \varepsilon^2 v_{xx} + 2\beta v + \sigma\theta, \tag{31}$$

$$\tau_\theta\theta_{tt} + \lambda\tau_\theta v_{tt} + \theta_t + \lambda v_t = D\theta_{xx} \tag{32}$$

coupled with

$$v_t = G_0[v] \quad \text{at} \quad x = 0, \quad v_t = G_1[v] \quad \text{at} \quad x = l, \tag{33}$$

$$\theta_t = \Upsilon_0[\theta] \quad \text{at} \quad x = 0, \quad \theta_t = \Upsilon_1[\theta] \quad \text{at} \quad x = l, \tag{34}$$

where τ_v, τ_θ are the corresponding relaxation times. We will look for a solution of these equations in the form of travelling waves, namely,

$$v(x, t) = v(s),\ \theta(x, t) = \theta(s),\ \text{where } s = t - x/V. \tag{35}$$

Substituting (35) into (31),(32), we get that

$$\left(\tau_v - \frac{\varepsilon^2}{V^2}\right)v'' + v' - 2\beta v = \sigma\tau_v\theta' + \sigma\theta, \tag{36}$$

$$\left(\tau_\theta - \frac{D}{V^2}\right)\theta'' + \theta' = -\lambda\tau_\theta v'' - \lambda v'. \tag{37}$$

Here, $\beta = \chi - \chi_c$ is the interaction energy between atoms of type A and B, χ_c is an energy of decomposition of a disordered phase on two ordered phases. By (36), (37) we deduce that

$$\alpha_0 v'''' + \alpha_1 v''' + \alpha_2 v'' + \alpha_3 v' = 0 \text{ if } \tau_\theta - \tau_v \neq \tfrac{D}{V^2}, \tag{38}$$

$$\tilde{\alpha}_1 v''' + \tilde{\alpha}_2 v'' + \tilde{\alpha}_3 v' = 0 \text{ if } \tau_\theta - \tau_v = \tfrac{D}{V^2}, \tag{39}$$

where

$$\alpha_0 = (\tau_v - \tfrac{\varepsilon^2}{V^2})(\tau_\theta - \tfrac{D}{V^2}),\ \alpha_1 = \tau_v - \tfrac{\varepsilon^2}{V^2} + \tau_\theta - \tfrac{D}{V^2} + \sigma\lambda\tau_v\tau_\theta,$$
$$\alpha_2 = 1 + \sigma\lambda(\tau_v + \tau_\theta) - 2\beta(\tau_\theta - \tfrac{D}{V^2}),\ \alpha_3 = \sigma\lambda - 2\beta,$$
$$\tilde{\alpha}_1 = \tau_v - \tfrac{\varepsilon^2}{V^2},\ \tilde{\alpha}_2 = 1 + \sigma\lambda\tau_\theta,\ \tilde{\alpha}_3 = \sigma\lambda - 2\beta.$$

Next, for simplicity, we will consider the case $V^2 = \frac{D}{\tau_\theta} = \frac{\varepsilon^2}{\tau_v}$ only.

4. Asymptotic solutions for the Penrose-Fife equations

4.1. Asymptotic solutions for the order parameter

If $V^2 = \frac{D}{\tau_\theta} = \frac{\varepsilon^2}{\tau_v}$ then from (38) we obtain that

$$\sigma\lambda\tau_v\tau_\theta v''' + (1 + \sigma\lambda(\tau_v + \tau_\theta))v'' + (\sigma\lambda - 2\beta)v' = 0. \tag{40}$$

By (40) we deduce that

$$v''' + a_0 v'' + a_1 v' = 0,\ \text{where } a_0 = \tfrac{1+\sigma\lambda(\tau_v+\tau_\theta)}{\sigma\lambda\tau_v\tau_\theta},\ a_1 = \tfrac{\sigma\lambda-2\beta}{\sigma\lambda\tau_v\tau_\theta}. \tag{41}$$

Integrating (41) from $s = t$ to $s = t - l/V$, we arrive at

$$v''(t) + a_0 v'(t) + a_1 v(t) = v''(t - l/V) + a_0 v'(t - l/V) + a_1 v(t - l/V), \tag{42}$$

whence, taking into account the boundary conditions (33), we get

$$G_0'[v(t)]G_0[v(t)] + a_0 G_0[v(t)] + a_1 v(t) =$$
$$G_1'[v(t - l/V)]G_1[v(t - l/V)] + a_0 G_1[v(t - l/V)] + a_1 v(t - l/V). \tag{43}$$

Let us denote by $\tilde{G}_0 := G_0'G_0 + a_0 G_0 + a_1 Id$, $\tilde{G}_1 := G_1'G_1 + a_0 G_1 + a_1 Id$, where Id is the identity map. Then from (43) we find the following difference equation

$$v(t) = G[v(t - l/V)],\ \text{where } G := \tilde{G}_0^{-1} \circ \tilde{G}_1. \tag{44}$$

On the other hand, integrating (41) on s, we arrive at

$$\begin{aligned} v(s) &= k_1 + k_2 e^{\lambda_1 s} + k_3 e^{\lambda_2 s} \text{ if } a_0 - 4a_1 \neq 0, \\ v(s) &= k_1 + k_2 e^{-\frac{a_0}{2}s} + k_3 s e^{-\frac{a_0}{2}s} \text{ if } a_0 - 4a_1 = 0 \end{aligned} \tag{45}$$

$\forall\, k_i \in \mathbb{R}$, where

$$\lambda_1 = \frac{-a_0 \pm \sqrt{a_0^2 - 4a_0 a_1}}{2}.$$

So, (45) forms admissible class of initial functions for difference equation (44), i. e.

$$v_0(t) = k_1 + k_2 e^{\lambda_1 t} + k_3 e^{\lambda_2 t} \text{ if } a_0 - 4a_1 \neq 0,$$

$$v_0(t) = k_1 + k_2 e^{-\frac{a_0}{2} t} + k_3 t e^{-\frac{a_0}{2} t} \text{ if } a_0 - 4a_1 = 0$$

for all $t \in [-l/V, 0)$.

For example, consider the boundary conditions (33) in the form

$$v_t = \alpha\, v \text{ at } x = 0, \quad v_t = f(v) \text{ at } x = l, \tag{46}$$

where $f(v)$ satisfies $f(v)(f'(v) + a_0) = (\alpha(\alpha + a_0) + a_1)(v^2 + \delta) - a_1 v$. Here $\alpha(\alpha + a_0) + a_1 \neq 0$ and δ are arbitrary parameters, then (44) is reduced to the logistic equation:

$$v(t) = v^2(t - l/V) + \delta. \tag{47}$$

It can be shown (see [18, 29]) that solutions of this equation tend to $2^N l/V$ — periodic function $p_1(t) \in P^+$ with a finite or an infinite number of discontinuity points $t^* \in \Gamma$ on a period as $t \to +\infty$, where P^+ is a set of attractive circles of a map $G : I \to I$, N is a common multiple of the attractive circles.

Now, we show what happens, for example, if we linearise boundary condition (33) at a disordered state $v = 0$. By (33) we arrive at

$$v_t(0, t) = G_0[0] + G_0'[0]v(0, t), \quad v_t(l, t) = G_1[0] + G_1'[0]v(l, t). \tag{48}$$

In this case, similar to (44) we get the following linear difference equation:

$$v(t - l/V) = m_1 v(t) + m_2, \tag{49}$$

where

$$m_1 = \frac{G_0'[0](G_0'[0]+a_0)+a_1}{G_1'[0](G_1'[0]+a_0)+a_1}, \ m_2 = \frac{G_0[0](G_0'[0]+a_0)-G_1[0](G_1'[0]+a_0)}{G_1'[0](G_1'[0]+a_0)+a_1}.$$

Equation (49) has a general solution

$$v(t) = \Theta(t) m_1^{-\frac{V}{l} t} + \frac{m_2}{1-m_1} \text{ if } m_1 \neq 1, \text{ and } v(t) = \Theta(t) - \frac{V}{l} m_2\, t \text{ if } m_1 = 1, \tag{50}$$

where $\Theta(t)$ is an arbitrary l/V-periodic function. So, the linearised boundary conditions give us very simple asymptotic behaviour.

4.2. Asymptotic solutions for temperature

If $V^2 = \frac{D}{\tau_\theta} = \frac{\varepsilon^2}{\tau_v}$ then by (36), (37) we deduce that

$$\theta'' + b_1\theta' + b_2 v' = 0, \text{ where } b_1 = \frac{1+\sigma\lambda\tau_\theta}{\sigma\lambda\tau_v\tau_\theta}, \ b_2 = \frac{1+2\beta\tau_\theta}{\sigma\tau_v\tau_\theta}. \tag{51}$$

Subtracting (51) at $s = t - l/V$ from (51) at $s = t$, we arrive at

$$\theta''(t) - \theta''(t - l/V) + b_1[\theta'(t) - \theta'(t - l/V)] + b_2[v'(t) - v'(t - l/V)] = 0. \tag{52}$$

Taking into account the boundary conditions (34) and equation (44), we get

$$\Upsilon_0'[\theta(t)]\Upsilon_0[\theta(t)] + b_1\Upsilon_0[\theta(t)] = \Upsilon_1'[\theta(t-l/V)]\Upsilon_1[\theta(t-l/V)] + b_1\Upsilon_1[\theta(t-l/V)] - b_2(G_0\circ G[v(t-l/V)] - G_1[v(t-l/V)]). \quad (53)$$

Let us denote by $\tilde{\Upsilon}_0 := \Upsilon_0'\Upsilon_0 + b_1\Upsilon_0$, $\tilde{\Upsilon}_1 := \Upsilon_1'\Upsilon_1 + b_1\Upsilon_1$, and $\tilde{G} := G_1 - G_0\circ G$. Then from (53) we find the following difference equation

$$\theta(t) = \tilde{\Upsilon}_0^{-1}\circ(\tilde{\Upsilon}_1[\theta(t-l/V)] + b_2\tilde{G}[v(t-l/V)]). \quad (54)$$

On the other hand, integrating (51) on s, we get

$$\theta(s) = k_4e^{-b_1s} - \tfrac{k_1b_2}{b_1} - \tfrac{k_2b_2}{b_1+\lambda_1}e^{\lambda_1 s} - \tfrac{k_3b_2}{b_1+\lambda_2}e^{\lambda_2 s}\ \forall\, k_i\in\mathbb{R},\ a_0 - 4a_1 \neq 0, \lambda_i \neq -b_1, \quad (55)$$

where k_1, k_2, k_3 are from (45). Thus, (55) provides admissible class of initial functions for difference equation (54), i. e. $\theta_0(t) = k_4e^{-b_1t} - \frac{k_1b_2}{b_1} - \frac{k_2b_2}{b_1+\lambda_1}e^{\lambda_1 t} - \frac{k_3b_2}{b_1+\lambda_2}e^{\lambda_2 t}$ for all $t\in[-l/V, 0)$.

For example, if $b_2 = 0$ and $\Upsilon := \tilde{\Upsilon}_0^{-1}\circ\tilde{\Upsilon}_1 : I \to I$ is structurally stable hyperbolic map then again we obtain the same difference equation to (44). It can be shown (see [18, 29]) that solutions of this equation tend to periodic piecewise constant function with a finite or an infinite number of discontinuity points on one period as $t\to+\infty$. If $b_2 \neq 0$ then we have to consider the coupled system of difference equations.

4.3. Example

In the general situation, we do not have any classical theory to apply. Therefore we will study one of simple examples to illustrate some possible scenarios of asymptotic behaviour of solutions. Consider the boundary conditions (33), (34) in the form

$$v_t = \alpha\, v \text{ at } x = 0,\quad v_t = \beta\, v \text{ at } x = l, \quad (56)$$

$$\theta_t = \gamma\,\theta \text{ at } x = 0,\quad \theta_t = g(\theta) \text{ at } x = l, \quad (57)$$

where $g(\theta)$ satisfies $g(\theta)(g'(\theta) + b_1) = \gamma(\gamma+b_1)(\theta^2+\mu)$. Here $\gamma \neq \{0, -b_1\}$, $\alpha(\alpha+a_0)+a_1 \neq 0$ and μ are arbitrary parameters. Then the system of difference equations (44), (54) are reduced to

$$\theta(t) = \theta^2(t-l/V) + a\,v(t-l/V) + \mu,\quad a = \tfrac{b_2(\alpha-\beta)(\alpha\beta-a_1)}{\gamma(\gamma+b_1)(\alpha(\alpha+a_0)+a_1)}, \quad (58)$$

$$v(t) = b\,v(t-l/V),\quad b = \tfrac{\beta(\beta+a_0)+a_1}{\alpha(\alpha+a_0)+a_1}. \quad (59)$$

Note that $\alpha = \beta$ then (58), (59) reduces to the following uncoupled system:

$$\theta(t) = \theta^2(t-l/V) + \mu,\quad v(t) = v(t-l/V). \quad (60)$$

If $|b| < 1$ then the map

$$\hat{f}_\mu : (\theta, v) \mapsto (\theta^2 + v + \mu, b\,v) \quad (61)$$

describes all trajectories of the dynamical system attracted by a line $v = 0$. Thus asymptotic behaviour of equation (58) is determined by properties of the one-dimensional logistic map

$$f_\mu : \theta \mapsto \theta^2 + \mu \quad (62)$$

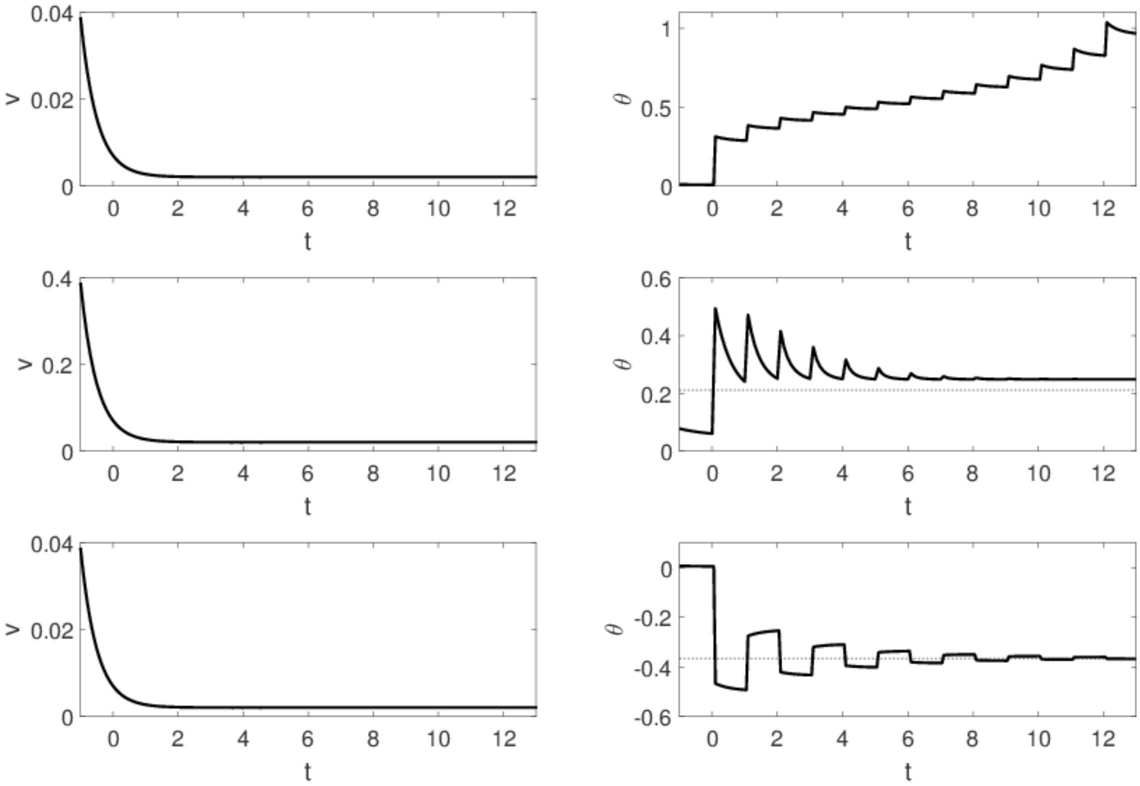

Figure 1. The upper pictures illustrate convergence of $v(t)$ to zero and divergence of $\theta(t)$ for $\mu = 0.28 > 1/4$, initial data $v(t) = 0.002 + 0.005\exp(-2t)$, $\theta(t) = 0.005 + 0.001\exp(-t)$, $b = 1/2$, and $l/V = 1$. The middle pictures illustrate convergence of $v(t)$ to zero and convergence from above of $\theta(t)$ to $\theta_1 \approx 0.15$ (dashed line) for $\mu = 1/8 < 1/4$, initial data $v(t) = 0.02 + 0.05\exp(-2t)$, $\theta(t) = 0.05 + 0.01\exp(-t)$, $b = 1/2$, and $l/V = 1$. The lower pictures illustrate convergence of $v(t)$ to zero and oscillating convergence of $\theta(t)$ to $\theta_1 \approx -0.37$ (dashed line) for $\mu = -1/2 > -3/4$, initial data $v(t) = 0.002 + 0.005\exp(-2t)$, $\theta(t) = 0.005 + 0.001\exp(-t)$, $b = 1/2$, and $l/V = 1$.

of the line $v = 0$ mapped into itself. For example, if $\mu > 1/4$ then $\theta(t) \to +\infty$ as $t \to \infty$ (see the upper picture on *Figure 1*) because there are no any fixed points. For $\mu = 1/4$, we have the saddle-node type fixed point $(1/2, 0)$. For $\mu < 1/4$, the map $\hat{f}_\mu$ has two fixed points $(\theta_1, 0) = (\frac{1-\sqrt{1-4\mu}}{2}, 0)$, $(\theta_2, 0) = (\frac{1+\sqrt{1-4\mu}}{2}, 0)$. As a result, we have a saddle-node bifurcation at $\mu = 1/4$.

If $\mu \in (-3/4, 1/4)$ then the point $(\theta_1, 0)$ is stable node type, and the point $(\theta_2, 0)$ is unstable saddle type (see *Figure 1*). The attractive region of the point $(\theta_1, 0)$ is an open unbounded region W at the plane (θ, v) with a boundary which contains the saddle point $(\theta_2, 0)$ of codimension one and separatrix of this point, and also countable set of curves. These curves are pre-image of the separatrix for iterations $\hat{f}_\mu^{-n}, n = 0, 1, \ldots$. The limit solution $f^\Delta(\theta, v)$ is (1) $(\theta_1, 0)$ as $(\theta, v) \in W$; (2) $(\theta_2, 0)$ as $(\theta, v) \in \partial W$; (3) $(+\infty, 0)$ as $(\theta, v) \notin \overline{W}$.

If $\mu \in (-5/4, -3/4)$ then the points $(\theta_{1,2}, 0)$ are saddle type and the map has attractive circle of period 2 formed by points $(\theta_3, 0) = (\frac{-1-\sqrt{-3-4\mu}}{2}, 0)$, $(\theta_4, 0) = (\frac{-1+\sqrt{-3-4\mu}}{2}, 0)$. In this case, we have solutions of *relaxation type* (see, *Figure 1*).

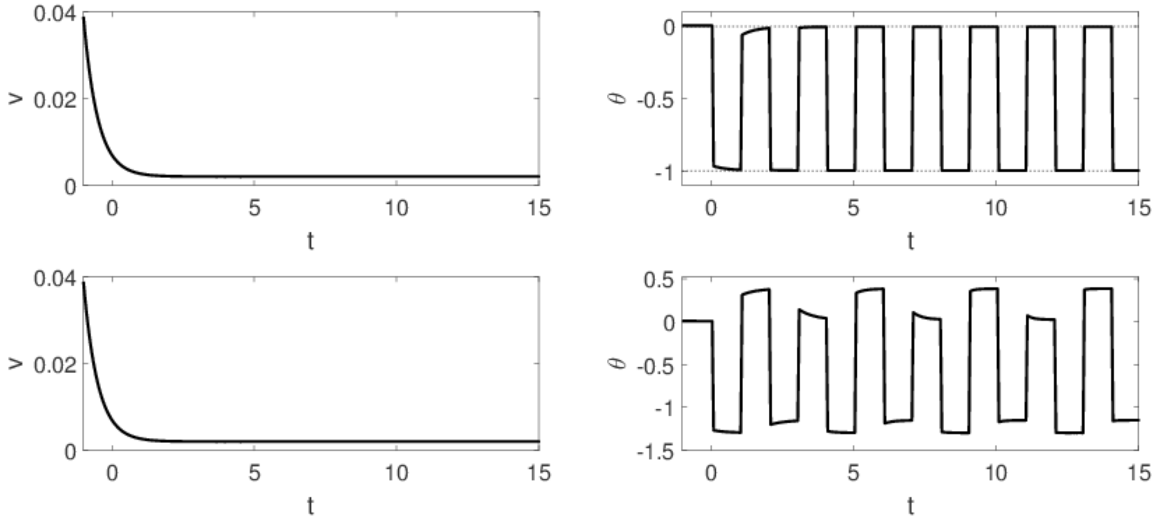

Figure 2. The upper pictures illustrate convergence of $v(t)$ to zero and convergence of $\theta(t)$ to piecewise constant function $\theta(t) = \theta_3 = -1,\ \theta(t) = \theta_4 = 0$ for $-5/4 < \mu = -1 < -3/4$, initial data $v(t) = 0.002 + 0.005\exp(-2t)$, $\theta(t) = 0.005 + 0.001\exp(-t)$, $b = 1/2$, and $l/V = 1$. The lower pictures illustrate convergence of $v(t)$ to zero and convergence of $\theta(t)$ to pre-turbulent type solution for $-1.401 \approx \mu^* < \mu = -1.3 <= 5/4$, initial data $v(t) = 0.002 + 0.005\exp(-2t)$, $\theta(t) = 0.005 + 0.001\exp(-t)$, $b = 1/2$, and $l/V = 1$.

If $\mu \in [\mu^*, -5/4]$, where $\mu^* = -1.401$, then the map f_μ has circles of periods $1, 2, 2^2, .., 2^n$ (ones of each periods!), where $2 \leqslant n = n(\mu) \to +\infty$ as $\mu \to \mu^*$. A circle of a period 2^n is attractive but another circles are repelling. In this case, a solution tends to a piecewise constant $2^N l/V$-periodic function as $t \to +\infty$, excluding the solution $\theta(t) = \theta_1$. The limit function has, at least, a countable set of points of discontinuities on a period. A number of oscillations of the limit solutions on each interval $(t, t + l/V)$ tends to a power function as $t \to +\infty$. We will call such solutions as solutions of *pre-turbulent type* (see Figure 2).

If $\mu \in (-7/4, \mu^*)$ then a set of non-wandering points of the map consists from attractive circle of a period 3 and Cantor set which represents closure of a set of points for repelling circles (see [17]). As a result, a solution tends to a $3l/V$-periodic function as $t \to +\infty$ (see Figure 3).

If $\mu \in \Lambda := (-2, -7/4)$ then bifurcations of solution accompanied by a change of periods with respect to the universal ordering (see [29, 30]):

$$1 \prec 2 \prec 2^2 \prec 2^3 \prec ... \prec 7 \cdot 2^2 \prec 5 \cdot 2^2 \prec 3 \cdot 2^2 \prec 7 \cdot 2 \prec 5 \cdot 2 \prec 3 \cdot 2 \prec ... \prec 7 \prec 5 \prec 3. \tag{63}$$

The period doubling bifurcations arise with universal velocity $\nu = 4.669$ and ones characterised by the universal relations of amplitudes of arising oscillations $\rho = 2.502$. From (63) it follows that for each m exists a map which has a circle of the period m' and one has not of circles of periods $m < m'$ as $m \prec m'$. For the period doubling bifurcations from (63) we get that $2^i \prec m$ for all $i \geq 0$ if $m \neq 2^i$, $i = 0, 1, 2, ...$ Next, define by $\mu[n]$ a least value of a parameter μ for which the map f_μ has a circle of a period n. Then for f_μ there is the ordering (see [30]):

$$\mu[1] \leq \mu[2] \leq \mu[4] \leq ... \leq \mu[5 \cdot 2] \leq \mu[3 \cdot 2] \leq ... \leq \mu[5] \leq \mu[3]. \tag{64}$$

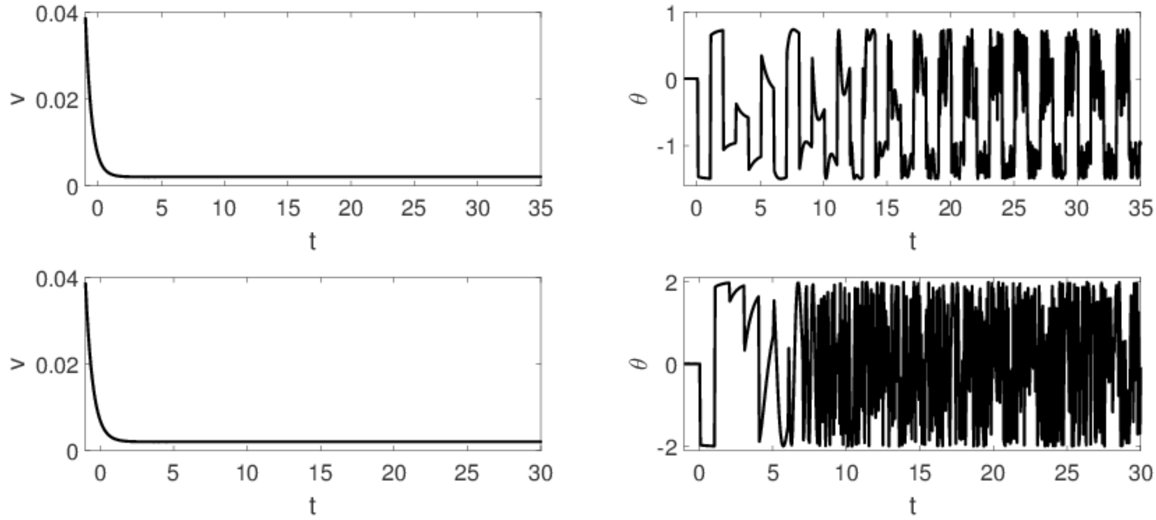

Figure 3. The upper pictures illustrate convergence of $v(t)$ to zero and convergence of $\theta(t)$ to $3l/V = 3$ periodic function for $-2 < \mu = -1.5 < \mu^*$, initial data $v(t) = 0.002+0.005\exp(-2t)$, $\theta(t) = 0.005+0.001\exp(-t)$, $b = 1/2$, and $l/V = 1$. The lower pictures illustrate convergence of $v(t)$ to zero and convergence of $\theta(t)$ to turbulent type solution for $\mu = -2$, initial data $v(t) = 0.002 + 0.005\exp(-2t)$, $\theta(t) = 0.005 + 0.001\exp(-t)$, $b = 1/2$, and $l/V = 1$.

Assume that

$$\Lambda_m^n = \{\mu \in \Lambda : f_\mu \text{ has a circle of a period } (2m+1)2^n\} \neq \emptyset, \quad m, n \in \mathbb{Z}^+, \tag{65}$$

and $\mu_m^n = \inf\ \Lambda_m^n$. Then from (64) we arrive at

$$\mu_0^0 \le \mu_0^1 \le \mu_0^2 \le \mu_3^1 \le \mu_2^1 \le \mu_1^1 \le ... \le \mu_3^0 \le \mu_2^0 \le \mu_1^0. \tag{66}$$

If $\mu = -2$ and initial function $\theta_0(t) : -2 \leqslant \theta_0(t) \leqslant 2\ \forall\, t \in [-l/V, 0)$ then a solution tends to a function, which values are equal to $[-2, 2]$ for any t, as $t \to +\infty$. It means that a solution of $\theta(t) = \theta^2(t - l/V) + \mu$ for any $t' < t''$ has a number of oscillations with the amplitude $[-2, 2]$ on interval $(t' + t, t'' + t)$ as $t \to +\infty$. The number of oscillations increases by 2 every time as time interval t increases by l/V and eventually goes to infinity. In this case, we will talk about limit solutions of *turbulent type* (see *Figure 3*). In addition, if $\mu < -2$ then all solutions become unbounded, except $\theta(t) = \theta_{1,2}$.

Note that the experiment which proves the existence of surface oscillating distributions of temperature has been done by Gao et al. (see, [9, Figure 2a]). The influence of latent heat on formation of surface heat structures in a pattern has been also explained in this article.

5. Discussion

5.1. Comparison with experiment

As an example of possible application of our results, we present some data from an experimental study of ordering (segregation) at the *CuAu* (100) surface. In [1], it is shown that *Au* enrichment in the top surface layer persists up to temperature far beyond the bulk order–disorder transition temperature.

The segregation, which happens below the bulk order-disorder transition temperature T_m, depends on compositional depth profile that gives information about the binding characteristics of such alloys. So, monotone profile indicates weak pair interaction between the two components but oscillating profile results from stronger pair interaction. Therefore it is useful to perform layer-selective composition analysis in the near-surface region. For example, for low-energy interaction there are no layers but for lager energy there arise three or more surface-layers (see [1, 4, 10, 20, 31, 32]). The theoretical study by Tersoff [32] for $CuAu$ (100) predicts Au segregation with oscillating segregation depth profile. So, Au rich layers can alternate with Au depleted layers. The average amplitude of these oscillations decreases while temperature increases. This average amplitude, according to Tersoff, decays exponentially into the bulk when value of T_m is above the bulk ordering transition temperature.

Thus, investigation of surface segregation requires layer composition analysis as a function of temperature. Such information can be obtained by the low-energy ion scattering beyond first layer chemical composition. The Cu and Au concentrations in the top layer are measured with He^+ ion scattering. Information about the first and second layer composition is obtained from Na^+ scattering spectra (see [1, Figure 2]). The spectra taken on the two different azimuthal directions show that Au is the dominant species in the top layer where both Cu and Au are detected in the second layer. The experimental results are well reproduced by the solutions of relaxation type with a unique point of 'discontinuities' on a period (see, Figure 1). So, the quantitative evaluation is possible.

The surface composition as a function of temperature range is obtained from quantitative evaluation of both, He^+ and Na^+ measurements. For this purpose, the Cu and Au concentrations in the surface layers were varied in the simulations until the best agreement between measured and calculated spectra were obtained.

To make it the crystal must be heated up to temperature of data points. At temperature $T < T_m$, the rapid cooling with liquid nitrogen must be necessary. Then at temperature $T < 0°C$ arise mixing in surface layers (or disordered state). The Au concentration at a neighbourhood $T = T_m$ is 0.95 of common concentration $Au + Cu = 1$ and decreases with higher temperature while the Cu concentration increases. As a result, there is the typical graphic form for oscillations of relaxation type with finite points of 'discontinuities' on a period. These oscillations describe the layers which are parallel to the (100) plane of the pattern.

Note that the remaining small Au concentration in the second layer indicates slight deviation from 'ideal' bulk temperature that qualitatively corresponds to the mathematical results. That is the oscillations are spatial-temporal piecewise constant distributions. Indeed, as noted in [1]: 'The asymmetric development of the Au concentration in the two layers relative to the bulk value X_{Vol}^{Au} is also assign of a damped oscillating concentration depth profile, which is similar to the case of Cu_3Au'. Thus, these results indicate on existence of a continuous phase transition in the surface region. Next, the asymmetric development of the Au concentration in the two layers which are relative to the bulk value X of the concentration Au_{Vol} is a sign of a damped oscillating concentration depth profile that are similar to the case of Cu_3Au [5, 24].

5.2. *Physical sense of boundary conditions*

At higher temperatures gradual desegregation is observed, i. e. decreasing of the Au concentration in the first layer accompanied by increasing Au concentration in the second layer. The degree of desegregation can be used to estimate the segregation energy ΔH. The Langmuir-McLean relation should be applied [23] to describe temperature dependence of the concentration X of the segregating components as

$$\frac{X^{surface}}{1 - X^{surface}} = \frac{X^{bulk}}{1 - X^{bulk}} e^{\frac{\Delta H}{k_B T}}, \tag{67}$$

where k_B is the Stefan-Boltzmann constant. For example, if $\frac{\Delta H}{k_B T} \ll 1$ then the solutions of the Penrose-Fife equations are determined in main by the boundary conditions, i. e. by the surface segregation energy. Thus, the cooling of a crystal with impurity leads to the formation of meta-stable states (or a number of clusters) which contain defects. These states are long lived (or meta-stable). Note that the crystallization in the bulk is difficult to identify but the crystallization at the surface can be determined by using of scanning tunneling microscope [5, 24].

Further, let us consider an example of simplest dynamic boundary conditions which are due to surface defects. If $T > T_m$, then positions of impurities are not correlated. But below T_m defects are correlated so that the rate of change of the order parameter v is proportional to v^2. It leads to phenomenon that if $T < T_m$, then defects are structured in clusters, and one would expect an increase in the number of defect fluctuations. In $1D$ approximation, the radiuses of clusters and its density may be described by distributions of relaxation type. Such distributions are captured by the boundary condition

$$\frac{\partial v}{\partial t} = kv^2 + \mu, \quad k, \mu \in \mathbb{R} \tag{68}$$

at the left wall that confines the binary alloy in the liquid state, and the same linear boundary conditions at the right wall. In a similar way, one can construct a special dynamic boundary conditions for the temperature, or even more complex boundary conditions, which are connected the order parameter and temperature in some nonlinear way. To conclude, we note that the dynamic boundary conditions were previously discussed in [13] for the binary alloys. At first, this type of boundary conditions was considered for polymer mixtures by Binder et al. [2, 25]. The Cahn-Hilliard equation in $3D$ geometry with dynamic boundary conditions was studied in [13], where $3D$-wave structures were obtained for the unit cube domain. These results can also be applied to the Penrose-Fife equations.

6. Conclusion

We consider the self-organization phenomenon in a binary alloy with memory which is in the disordered state and confined by the two flat walls. This problem postulated as an initial boundary value problem for the hyperbolic Penrose-Fife equations with dynamic boundary conditions. Such type model describes evolution of order parameter and temperature in a binary alloy. It is shown that the solutions of the problem can be represented in the form of travelling waves. This allows us to reduce the PDE problem to the initial value problem for two difference equations with continuous time delay. In particular case when these equations have special quadratic form, it is proved that asymptotic solutions satisfy to the Sharkovsky ordering. These solutions have the finite or infinite points of discontinuities on a period. As a result, we get the oscillating solutions for order parameter and temperature. Thus, behaviour of order parameter and temperature about the walls, due to the dynamic boundary conditions, leads to appearance of surface induced spatia-temporal oscillations into a bulk.

Conflict of interest

All authors declare no conflicts of interest in this paper.

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