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The surface-induced spatial–temporal structures in confined binary alloys

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HIGHLIGHTS

- The new model is derived for surface-induced ordering in confined binary alloys.
- Effects of the "memory" on the ordering of atoms are analysed.
- Three different types of attractor's elements are obtained.

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ABSTRACT

This paper examines surface-induced ordering in confined binary alloys. The hyperbolic initial boundary value problem (IBVP) is used to describe a scenario of spatiotemporal ordering in a disordered phase for concentration of one component of binary alloy and order parameter with non-linear dynamic boundary conditions. This hyperbolic model consists of two coupled second order differential equations for order parameter and concentration. It also takes into account effects of the "memory" on the ordering of atoms and their densities in the alloy. The boundary conditions characterize surface velocities of order parameter and concentration changing which is due to surface (super)cooling on walls confining the binary alloy. It is shown that for large times there are three classes of dynamic non-linear boundary conditions which lead to three different types of attractor's elements for the IBVP. Namely, the elements of attractor are the limit periodic simple shock waves with fronts of "discontinuities" Γ. If Γ is finite, then the attractor contains spatiotemporal functions of relaxation type. If Γ is infinite and countable then we observe the functions of pre-turbulent type. If Γ is infinite and uncountable then we obtain the functions of turbulent type.

1. Introduction

In this paper, we study the initial boundary value problem for the following equations of hyperbolic type

$$\mu\frac{\partial^2\varphi}{\partial t^2}+\frac{\partial\varphi}{\partial t}=D_1\frac{\partial^2\varphi}{\partial x^2}-a_1\varphi-a_2c-\mu\left(a_1\frac{\partial\varphi}{\partial t}+a_2\frac{\partial c}{\partial t}\right), \tag{1}$$

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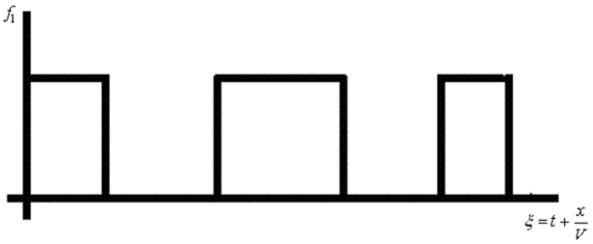

Fig. 1. Typical surface-induced asymptotic distributions of order parameter at a neighbourhood of disordered phase.

$$\nu\frac{\partial^2 c}{\partial t^2} + \frac{\tau_c}{\tau_\varphi}\frac{\partial c}{\partial t} = D_2\frac{\partial^2 c}{\partial x^2} + D_3\frac{\partial^2 \varphi}{\partial x^2}, \tag{2}$$

with initial data

$$c(x,0) = c_0(x), \qquad \frac{\partial c}{\partial t}(x,0) = c_1(x), \qquad \varphi(x,0) = \varphi_0(x), \qquad \frac{\partial \varphi}{\partial t}(x,0) = \varphi_1(x), \tag{3}$$

coupled with nonlinear dynamic boundary conditions

$$\frac{\partial \varphi}{\partial t}(0,t) = F_0(\varphi(0,t), c(0,t)), \qquad \frac{\partial \varphi}{\partial t}(l,t) = F_l(\varphi(l,t), c(l,t)), \tag{4}$$

$$\frac{\partial c}{\partial t}(0,t) = G_0(\varphi(0,t), c(0,t)), \qquad \frac{\partial c}{\partial t}(l,t) = G_l(\varphi(l,t), c(l,t)), \tag{5}$$

and the Neumann ones

$$\frac{\partial \varphi}{\partial x}(0,t) = \frac{\partial \varphi}{\partial x}(l,t) = 0, \qquad \frac{\partial c}{\partial x}(0,t) = \frac{\partial c}{\partial x}(l,t) = 0, \tag{6}$$

where $\varphi(x,t)$ is an order parameter and $c(x,t)$ is a concentration and $F_k,\ G_k : I \to I$ are the given functions, where I is an open bounded interval. These functions characterize the velocities of surface concentration and order parameter changing and they depend on temperature as a parameter. They may also depend on surface barriers and may describe, in particular, the process of bubbles nucleation in a new partially ordered phase originated from disordered state by surface supercooling (bubble nucleation process becomes faster at higher temperatures). The parameters $D_i,\ a_i$ will be defined in the next section. Note that the parabolic case ($\mu = \nu = 0$) of the system (1)–(2) was considered in Ref. [1], and a system similar to (1)–(2) was studied in Ref. [2]. In particular, in Ref. [1] the authors consider the solute trapping in a Si–As alloy during rapid solidification and compare the hyperbolic and parabolic models with finite interface dissipation.

The problem (1)–(6) describes the process of surface-induced nucleation of bubbles into the bulk by modelling the distributions of perturbations of the order parameter φ at the neighbourhood of the disordered state $\varphi = 0$, and, correspondingly, the distributions of concentration in the neighbourhood of the point $c = 1/2$. We investigate the memory effects presented in the asymptotic behaviour of the order parameter and concentration in confined binary alloys. We show that these effects are completely different for unbounded and bounded mixtures. For unbounded mixtures, as it was shown by Galenko et al. (see Refs. [3,4]), the hyperbolic model should be used for short initial times of the order parameter (concentration) evolution and a parabolic model describes long time behaviour. Particularly, see for details [4], damped oscillations arise in the hyperbolic Cahn–Hilliard model at the initial stage of the evolution. These oscillations tend to disappear at later times. As a result, the hyperbolic evolution admits reduction to the dissipative parabolic one. However, this transition from the hyperbolic type to parabolic type does not happen if we consider the confined binary systems coupled with dynamic nonlinear boundary conditions. In this case, the boundary conditions (i.e. nucleation of surface bubbles penetrating into the bulk) result into a new type of oscillations with non-decaying amplitudes. Hence, the evolution of the order parameter stays in hyperbolic regime even at later times and it has a periodic piece-wise constant structure (see, Fig. 1).

Numerical simulations for periodic or Neumann boundary conditions can be found, for example, in Refs. [5–11]. These are the spatial–temporal bulk oscillations with amplitudes decaying exponentially as time goes to infinity. For example, the diffusion model has been considered in Refs. [1,12] to model the micro-structural evolution of Ni solid solution. For binary alloy Sn–Pb, the evolution of the order parameter was simulated to study processes of dendrite growth, spinodal decomposition and so on (see, [13]). Note that dendrite growth occurs from a melt under super-cooling. The structure of the melt is characterized by short-range order (SRO) parameter field and the structure of a dendrite is characterized by long-range order (LRO) parameter field. Moreover, there is also a concentration field for one particular component of the binary alloy. These fields are used to describe distributions of this component of binary mixture and the $L1_2$ order phase structure. So, in Ref. [12] the micro-structures of Ni–Al were studied for the fixed temperature ($\sim$1000 K) regime by numerical simulations. Particularly, one can find in Ref. [12, Fig. 9] that there are two equilibrium ordered phases and these phases are both included into the disordered phase. As shown in Ref. [12], the total energy of the system decreases in time except for the case of the nucleation state.