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Numerical Analysis of Eguchi-Oki-Matsumura Model (for Phase Separation)

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Abstract

In thermodynamics, phase separations in binary alloys are interesting phenomena. J.W.Cahn and J.E.Hilliard introduced the free energy and derived the famous Cahn-Hilliard equation to analyze the spinodal decomposition. The relative minimizers for the free energy are very interesting in mathematics, especially whose instability gives difficult problems to makers of several products using alloys.

T. Eguchi, K. Oki, and S. Matsumura introduced the degree of order in binary alloys adding to the concentration of components to investigate the kinetics of phase separations. Using this model, we shall show that the local concentration begins to diverge by small perturbations in the degree of order though the distribution at the beginning is homogeneous.

1 Introduction

We introduce the Eguchi-Oki-Matsumura equation describing a phase separation for a substitutional binary alloy $A_{1-m}B_{1+m}$ consisting of A and B atoms filled in a vessel. In the continuum theory, the local concentration u is first introduced to be conserved as

$$\frac{1}{|\Omega|}\int_{\Omega} u(t,x)\,dx = m, \tag{1}$$

where Ω is a bounded domain in $\mathbb{R}^n, n = 1,2,3$, with the smooth boundary $\partial\Omega$. Next the local degree of order v is introduced to describe the thermodynamic potential of this system

as

$$F(u,v) = \int_\Omega (f(u,v) + \frac{1}{2}H|\nabla u|^2 + \frac{1}{2}K|\nabla v|^2)\, dx. \tag{2}$$

Here, $f(u,v)$ is the density of the bulk free energy,

$$f(u,v) = \frac{1}{2}au^2 - \frac{1}{2}bv^2 + \frac{1}{4}b_1v^4 + \frac{1}{2}gu^2v^2, \tag{3}$$

where a, b_1, g are positive constants, and b is a physical parameter depending on the temperature such as to be positive only below the critical one. And K, H are the surface energy per unit area considered to be positive constants. Then the equations of equilibrium state are given as follows,

$$\frac{\partial f(u,v)}{\partial u} = \mu, \frac{\partial f(u,v)}{\partial v} = 0, \tag{4}$$

where μ is a chemical potential.

Hence we obtain the kinetic equations for u and v,

$$L^{-1}\frac{\partial u}{\partial t} = -\nabla^2(H\nabla^2 u - \frac{\partial f(u,v)}{\partial u}), \tag{5}$$

$$\frac{\partial v}{\partial t} = K\nabla^2 v - \frac{\partial f(u,v)}{\partial v} \qquad \text{in } \Omega, \tag{6}$$

where L is the coefficient of diffusion speed of the material to one of the degree of order. These equations are analyzed with the boundary conditions

$$\nu \cdot \nabla u(t) = 0, \tag{7}$$

$$\nu \cdot \nabla^3 u(t) = 0, \tag{8}$$

$$\nu \cdot \nabla v(t) = 0 \qquad \text{on } \partial\Omega, \tag{9}$$

such that the equation (1) is satisfied, and the initial conditions

$$u(0) = u_o, \tag{10}$$

$$v(0) = v_o \qquad \text{in } \Omega. \tag{11}$$

2 Mathematical Results

We can show the well posedness of the problem based on the Eguchi-Oki-Matsumura model.

Theorem 1 *For any* $T > 0$ *and any* $(u_o, v_o) \in L_2 \times (L_2 \cap L_4)$, *there exist a solution* $(u, v) \in C_w(0, T; L_2)$ *satisfying*

$$u \in L^\infty(0,T;L_2) \cap L_2(0,T;H^1),$$

$$v \in L^\infty(0,T;L_2 \cap L_4) \cap L_2(0,T;V) \cap L_6(0,T;L_6)$$

$$\frac{1}{L}\frac{d}{dt}(u,\phi) = -H(\nabla^2 u, \nabla^2 \phi) + (\frac{\partial f(u,v)}{\partial u}, \nabla^2 \phi) \tag{12}$$

$$\forall \phi \in H^2(\Omega), \nu \cdot \nabla u = 0 \text{ on } \partial\Omega$$

$$\frac{d}{dt}(v,\psi) = -K(\nabla v, \nabla \psi) + (\frac{\partial f(u,v)}{\partial v}, \psi) \quad \forall \psi \in H^1(\Omega) \tag{13}$$

$$(u(0), v(0)) = (u_o, v_o). \tag{14}$$

2.1 The solutions homogeneous in space

If the distributions u, v are constant in space, the equations (5-6) is reduced to

$$\dot{u} = 0, \tag{15}$$

$$\dot{v} = (gu^2 + v^2 - b)v, \tag{16}$$

where $\dot{u}, \dot{v}$ denote $du/dt, dv/dt$. Since we have $u(t) = m$, let $\beta = b - gm^2$. Then we have, if $\beta = 0$,

$$v(t) = \frac{v_o}{(2t{v_o}^2 + 1)^{\frac{1}{2}}}, \tag{17}$$

or otherwise

$$v(t) = v_o(\frac{\beta}{{v_o}^2 - ({v_o}^2 - \beta)\exp^{-2\beta t}})^{\frac{1}{2}}. \tag{18}$$

In more realistic situations, the quantity b increases as the alloy gradually cooled down. So the growth, or changing of b in time must be considered strictly. However, in this paper, we separate the heat convection in the alloy from the model of phase separations.

First, if the temperature of the binary alloy is still high enough for $\beta \leq 0$, then we have

$$\lim_{t\to\infty} v(t) = 0.$$

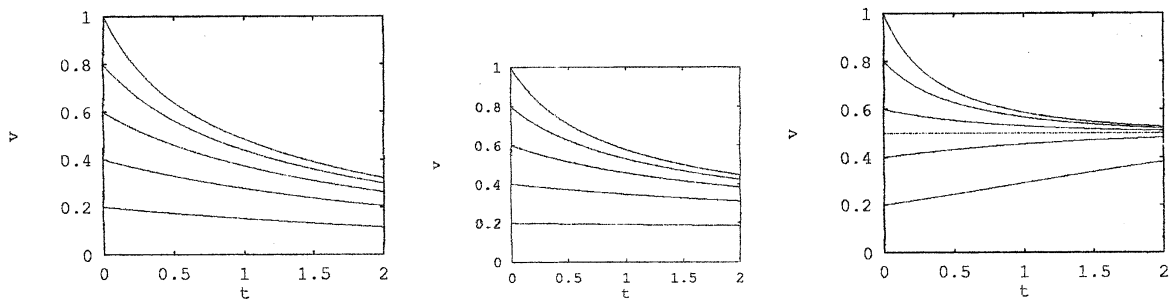

Figure 1: Evolution of homogeneous solutions, $\beta < 0, \beta = 0, \beta > 0$, respectively

Next, if the temperature is below the critical value such that $b > 0$, there exist other situations such that

$$\lim_{t\to\infty} |v(t)| = \sqrt{\beta},$$

if $v(t) \neq 0$ at some t. In this case, $v(t) = 0$ still satisfy the equations (15-16), but it is unstable(Fig.2).

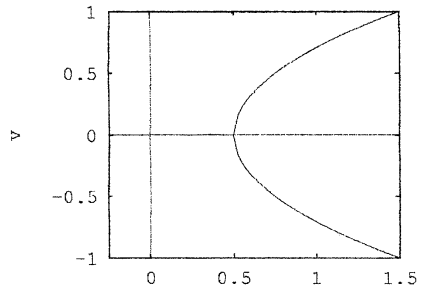

Figure 2: Bifurcation of uniform solutions $v(t)$ in b

As a stationary state of u and $|v|$, let

$$(\overline{u}(\beta), \overline{v}(\beta)) = \begin{cases} (m, 0) & (\beta \leq 0), \\ (m, \sqrt{\beta}) & (\beta > 0). \end{cases}$$

Then, we have

$$\lim_{t\to\infty} v(t) = \pm\overline{v}(\beta), \text{ or } 0,$$

in accordance with the sign of $v(0)$.

3 Problems of One-dimension in space

In this section, the problems of u and v depending on time t and only one direction x are studied. Then the equations (5-6) is reduced to

$$L^{-1}\dot{u} = -(Hu'' - (a + gv^2)u)'', \tag{19}$$

$$\dot{v} = Kv'' - (gu^2 + v^2 - b)v, \tag{20}$$

where u', u'', etc. denote $du/dx, d^2u/dx^2$, etc., respectively.

For the problem (19-20), there are not only homogeneous solutions described in the previous section, but also nonhomogeneous ones. In order to examine whether the homogeneous solutions are stable or not, and look for other solutions, numerical simulations are used.

3.1 Discretized Schemes

The equations (19-20) in the domain $(0, \infty) \times (0, 1)$ is discretized with forward differences in time and central differences in space. Let $x_k = k\Delta x, \Delta x = 1/n$, then the equations for approximations U_k of $u(t, x_k)$ and V_k of $v(t, x_k)$ are as following:

$$\begin{aligned} L^{-1}\frac{\overline{U}_k - U_k}{\Delta t} =& - H\frac{U_{k-2} - 4U_{k-1} + 6U_k - 4U_{k+1} + U_{k+2}}{\Delta x^4} \\ &+ \frac{(a + gV_{k-1}{}^2)U_{k-1} - 2(a + gV_k{}^2)U_k + (a + gV_{k+1}{}^2)U_{k+1}}{\Delta x^2}, \end{aligned} \tag{21}$$

$$\frac{\overline{V}_k - V_k}{\Delta t} = K\frac{V_{k-1} - 2V_k + V_{k+1}}{\Delta x^2} - (gU_k{}^2 + V_k{}^2 - b)V_k \tag{22}$$

$$(0 \le k \le n),$$

where $\overline{U_k}$ and $\overline{V_k}$ are the approximations at the next time step at $t + \Delta t$. The boundary conditions $u' = 0, u''' = 0$ are discretized as

$$U_{-2} = U_2,\ U_{-1} = U_1,\quad U_{n-1} = U_{n+1},\ U_{n-2} = U_{n+2}, \tag{23}$$

and $v' = 0$ is as

$$V_{-1} = V_1,\ V_{n-1} = V_{n+1}. \tag{24}$$

In numerical simulations taking constants as

$$L = 1/1024,\ H = K = 1/1000, m = 0.25, a = 0.25, g = 8, b_1 = 1,$$

the dependence of solutions on b, and the stability of the homogeneous states are studied.

3.2 Instability of the homogeneous solutions

In this subsection, we show that the homogeneous solutions are not stable if $\beta > 0$. For that purpose, initial conditions are perturbed slightly from the homogeneous solutions.

3.2.1 Zero solution $v = 0$

Taking initial conditions as

$$\begin{aligned} u(0,x) &= \quad m, \\ v(0,x) &= \epsilon\cos(\pi x) \quad \text{for small } |\epsilon|. \end{aligned}$$

The solutions, especially $u(t)$, are firstly going away from the initial state for all values of b. Then, $u(t)$ is converging to the constant function m if $\beta \leq 0$, then we may conclude that the homogeneous zero solution is stable. However, if $\beta > 0$, then the perturbation for

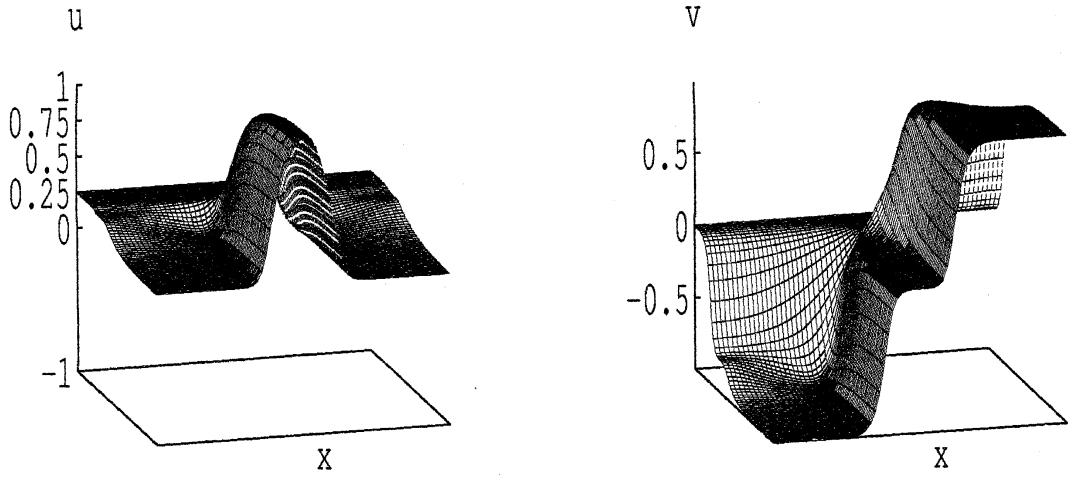

Figure 3: Behavior of $u(t,x), v(t,x)$ (evolving from behind)

v is expanding to the values near $\pm\sqrt{b}$, and it is followed by the separation of the values of u (which is observed as the phase separation phenomena). It is shown by mathematical analysis in the previous subsection 2.1. In Figure 3, the simulated results are shown in

the case of $b = 0.99($, therefore $\beta = 0.49$), $\epsilon = 0.001$, $\Delta t = 1/256$ and $\Delta x = 1/64$, while $0 \leq t \leq 128$.

3.2.2 Instability of $v = \sqrt{\beta}$

Taking a value of b such that $\beta > 0$, there exists the solution $(u, v) = (m, \sqrt{\beta})$. Therefore, it is important to simulate solutions starting from the initial states near that homogeneous solution as

$$\begin{aligned} u(0,x) &= m, \\ v(0,x) &= \sqrt{\beta} + \epsilon \cos(\pi x). \end{aligned}$$

For small ϵ such that $\epsilon^2 < \beta$, $v(0,x)$ is positive, and $v(t,x)$ is kept to be positive also. In this case, $v(t)$ approaches to a function oscillating between a number near $\sqrt{b}$ and another positive near zero. Then, oscillations of $u(t)$ appears according to ones of $v(t)$. In Figure 4, the simulated results are shown in the same parameters, while $0 \leq t \leq 4096$. However, the number of oscillations of $v(t)$ and $u(t)$ varies from one at first, to three secondly, and to one after a long time. Also other simulations result in the same solution having one oscillation, other than having many oscillations by symmetries.

4 Conclusion

In numerical simulations, we have observed that some homogeneous solutions are not stable in one-dimensional problems. Then, it is shown that the phenomena of phase separation in binary alloy are caused by perturbation only in the order parameter.

Since it is thought that the stationary problems in the E.O.M. model have many solutions stable or not, the structure of all solutions is left to be made clear.

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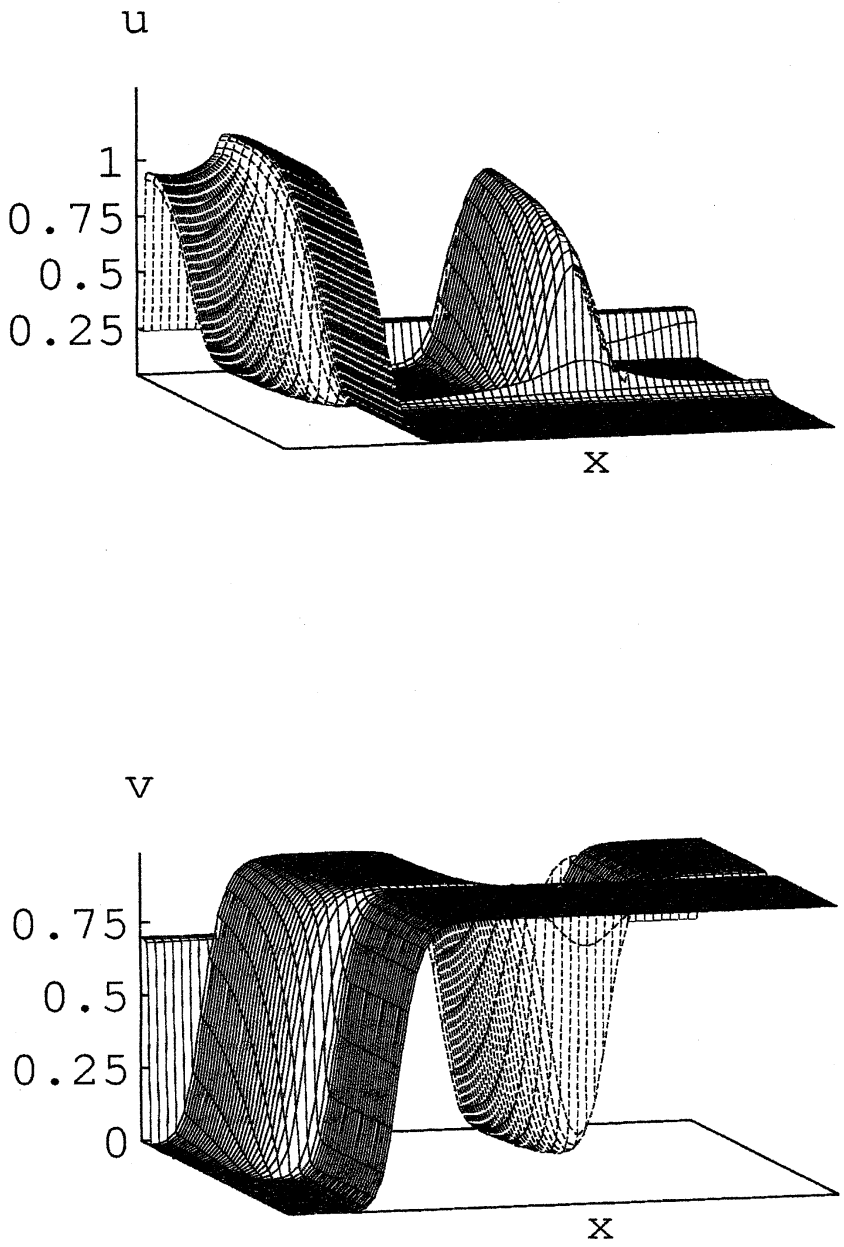

Figure 4: Behavior of $u(t,x), v(t,x)$

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