

# *An Analysis of Phase-Field Alloys and Transition Layers*

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## **Contents**

1. Introduction . . . . .	293
2. Mathematical Models of the Alloy Problem . . . . .	296
3. Asymptotic Analysis . . . . .	305
4. Interaction Between Dynamic and Static Transition Layers . . . . .	307
5. A Steady-State Problem with Constant Temperature . . . . .	315
6. A Partial Differential Equation System with Constant Temperature . . . . .	316
References . . . . .	328

## **Abstract**

A phase-field approach to binary alloys is studied. Formal asymptotics of the system of parabolic differential equations leads to new interface relations as part of a macroscopic model which arises in the limit of vanishing interface thickness. Under suitable conditions we prove that the phase-field system has a unique solution which converges to the limiting macroscopic solution. The concentration and phase are monotonic across the interface for a simplified system. Transition layers in concentration are induced due to the change in phase and the change in material diffusion across the interface. Excess impurities may be trapped as a consequence of these layers.

## **1. Introduction**

The dynamics of phase boundaries for pure material has been studied extensively, primarily by two avenues: sharp-interface models (e.g., [Cr] and references therein) and diffused-interface or phase-field models (e.g., [C1] and references therein). The sharp-interface models are generally macroscopic continuum models which stipulate basic equations, such as the heat equation in each phase, and impose

conditions on the interface (of zero thickness). A typical example is the surface tension and kinetics model (also called the modified Stefan model) in which a material in a spatial region  $\Omega \subset R^d$  is in one of two phases, e.g., liquid or solid, separated by an interface  $\Gamma \subset R^{d-1}$  satisfying the equations

$$C_V T_t = \nabla \cdot K_1 \nabla T \quad \text{in } \Omega \setminus \Gamma, \quad (1.1)$$

$$[T]_{\pm}^{\pm} = 0 \quad \text{on } \Gamma, \quad (1.2)$$

$$lv = -K_1 [\nabla T \cdot n]_{\pm}^{\pm} \quad \text{on } \Gamma, \quad (1.3)$$

$$[s]_E (T - T_M) = -\sigma(\alpha v + \kappa) \quad \text{on } \Gamma, \quad (1.4)$$

where  $T$  is (absolute) temperature,  $C_V$  is the specific heat per unit volume with units of energy/(volume · degree),  $K_1$  is the thermal conductivity with units of energy/(area · time · temperature gradient) = energy/(length <sup>$d-2$</sup>  · degree · time),  $l$  is the latent heat per unit volume with units of energy/mass,  $v$  is the normal velocity of the interface (positive if directed toward the liquid),  $n$  is the unit vector normal to the interface (pointing to the liquid),  $s$  is the entropy per unit volume with units of energy/(length <sup>$d$</sup>  · degree),  $[s]_E$  is the entropy difference in equilibrium per unit volume between the “+” phase and “−” phase,  $\kappa$  is the sum of principal curvatures at the point on  $\Gamma$ ,  $\sigma$  is the surface tension with units of energy/area = energy/length <sup>$d-1$</sup> ,  $\alpha$  is the relaxation scaling with units of time/length <sup>$2$</sup> ,  $T_M$  is the melting temperature, and  $[\cdot]_{\pm}^{\pm}$  denotes the jump between solid and liquid.

A dimensionless version of (1.1)–(1.4) uses a rescaled dimensionless temperature  $u$ , diffusivity  $D$ , and capillary length  $d_0$ , defined by

$$u \equiv \frac{T - T_M}{l/C_V}, \quad D \equiv \frac{K_1}{C_V}, \quad d_0 \equiv \frac{\sigma}{[s]_E l / C_V}, \quad (1.5)$$

so that the equations have the form

$$u_t = D \Delta u \quad \text{in } \Omega \setminus \Gamma, \quad (1.6)$$

$$[u]_{\pm}^{\pm} = 0 \quad \text{on } \Gamma, \quad (1.7)$$

$$v = -D [\nabla u \cdot n]_{\pm}^{\pm} \quad \text{on } \Gamma, \quad (1.8)$$

$$u = -d_0(\alpha v + \kappa) \quad \text{on } \Gamma. \quad (1.9)$$

In the special case when (1.9) is replaced by  $u = 0$ , one obtains the classical Stefan problem [Cr], which is the oldest mathematical model for a phase boundary. It is worth noting that (1.6)–(1.9) differs from the classical Stefan model in a much more fundamental way than the modification of an interface condition. In the classical Stefan model, the temperature alone specifies the phase, i.e., if  $u > 0$ , then the material is liquid at  $(x, t)$ , etc. However, the surface tension and kinetic model provides no such simple mechanism for determining phase, except by tracking the interface. Another way of stating this is that the classical Stefan model can be written in a weak formulation by means of a phase variable  $\phi^s$ , which is a Heaviside function of the (reduced) temperature, i.e.,  $\phi^s(u) = u^{-1}|u|$ . In the physically more realistic cases, this trivial dependence of phase on temperature must be replaced by a more complicated relationship. A natural method of accomplishing this within

the context of modern physics is by means of a free energy  $\mathcal{F} = \int_{\Omega} F dx$  which depends on temperature  $T$ , and a phase or order parameter  $\phi$ , which may be regarded as a microscopic fractional mass of one of the two phases. In most of the phase-field works,  $\phi$  is normalized so that  $\phi = 1$  corresponds to liquid and  $-1$  to solid. The heat equation (1.1) is replaced by an analogous energy balance law, the simplest of which is,

$$C_V T_t + \frac{1}{2} l \phi_t = K_1 \Delta T.$$

In equilibrium, the function  $\phi$  is a minimizer of the free energy so that  $\delta F / \delta \phi = 0$ . A standard idea of nonequilibrium statistical mechanics [HH] is that  $\phi$  returns to equilibrium with a “force” which is proportional to the extent to which it is out of equilibrium, so that  $\tau \phi_t = -\delta F / \delta \phi$  where  $\tau$  is a relaxation time. A typical free energy utilizes a Landau-type quadratic for  $\phi$ , so that in  $N$  dimensions we have

$$\mathcal{F}\{\phi, T\} = \int \left\{ \frac{\xi^2}{2} (\nabla \phi)^2 + \frac{1}{8a} (\phi^2 - 1)^2 - \frac{[s]}{2} (T - T_M) \phi \right\} dx, \quad (1.10)$$

where  $\xi$  is a length scale associated with the microscopic interaction strength,  $a^{-1}$  is a measure of the depth of the double-well,  $[s]_E$  is the entropy difference between phases in equilibrium and  $T_M$  is the melting temperature (see [C2] and references therein). Upon making the definitions of the macroscopic parameters

$$\varepsilon \equiv \xi a^{1/2}, \quad \sigma \equiv \frac{2}{3} \xi a^{-1/2}, \quad \alpha \equiv \frac{\tau}{\xi^2}, \quad (1.11)$$

where  $\varepsilon$  is a measure of the interface thickness and  $\sigma$  the surface tension, we can rewrite  $\mathcal{F}$  in terms of  $\varepsilon$  and  $\sigma$ , so that the dynamic equation for  $\phi$  is

$$\alpha \varepsilon^2 \phi_t = \varepsilon^2 \Delta \phi + \frac{1}{2} (\phi - \phi^3) + \varepsilon \frac{[s]_E}{3\sigma} (T - T_M). \quad (1.12)$$

This equation for  $\phi$  and  $T$  is coupled with the analogue of the heat equation (1.1), which in its simplest form is

$$C_V T_t + \frac{1}{2} l \phi_t = K_1 \Delta T. \quad (1.13)$$

The system (1.12) and (1.13) is a set of differential equations which describe the free-boundary problem (in the limit case) without the need for conditions on the interface, since the interface now consists of the set of points

$$\Gamma(t) \equiv \{x \in \Omega \mid \phi(x, t) = 0\}. \quad (1.14)$$

It is worth noting that the phase-field equations in the form (1.12), (1.13) identify all macroscopic variables such as  $[s]_E$ ,  $\sigma$ , etc., in the appropriate units. Also, the linearity with respect to  $\phi$  in the last term of  $\mathcal{F}$  expresses a linear approximation to entropy change across the interface. This choice of linearity implies that the roots  $\phi_{\pm}$  of the non-differentiated terms of the phase equation (1.12) are not fixed at  $\pm 1$ . For some purposes, it may be mathematically convenient to have  $\phi_{\pm}$  fixed at  $\pm 1$  [CC]. This is easily done by modifying the last term in (1.10). However, as noted

in [CJ], fixing the order parameter in the pure phase is incompatible with a more realistic phase diagram (e.g., a nontrivial pressure-density profile).

A theoretical link between the phase-field model (1.12) and (1.13) and sharp-interface models such as (1.6)–(1.9) was established by using formal matched asymptotics in [C1,2] and rigorously proved under various conditions in [CC, CF, S1,2]. A number of theorems have also been proved for the special case in which the phase equation (1.12) is considered independently for fixed  $T$  (see [ESS] and references therein). While the theoretical results are concerned with the limit  $\varepsilon \rightarrow 0$ , computations have shown that the phase-field equations exhibit an interface which is close to the sharp-interface problem even when  $\varepsilon$  is relatively large [CS].

In the present paper, we discuss a generalization of this model to the case of alloys. A related approach has been used in the isothermal case in [WBM1]. We will use a simplification of the set of equations which are derived in [CJ]. Our aim is to write the simplest system of equations of phase-field type which has the characteristic behavior of alloys and can be shown through asymptotic analysis to have the appropriate scaling and coefficients, and to present the rigorous proof in some special cases as the parameter  $\varepsilon \rightarrow 0$ .

The layout of this paper is as follows. In Section 2 we review the traditional models for alloys and present the phase-field approach to interface in binary mixtures. In Section 3 we perform an asymptotic analysis in order to derive the limiting sharp-interface problems (in the limit as interface thickness vanishes) which involve new interface relations and reduce to the traditional models in the limit of small concentration. In Section 4 we examine rigorously the question of the dynamic and static transition layers which are formed in the concentration variable. The interaction between these layers is the basis for the freezing of excess impurities in the solid. Finally, in Sections 5 and 6 we present a rigorous proof of some of the assertions of the asymptotics in one-dimensional space at constant temperature.

## 2. Mathematical Models of the Alloy Problem

### 2.1. The Alloy Problem

The problem of phase boundaries involving mixture of two materials (e.g., alloys or impurities) is of great practical interest and presents challenging theoretical issues which we review briefly in this section. We consider a substance (e.g., a binary alloy) consisting of a mixture of material A and material B, with concentration  $c(x, t) \in (0, 1)$  denoting the fraction of material A in the mixture. Two aspects of this problem are particularly fascinating from a mathematical perspective: (a) There is a jump in the concentration itself, and not just in the gradient, as in temperature. (b) The diffusion of impurities is generally much smaller in the solid phase compared with the liquid, and leads to partly degenerate equations.

An understanding of (a) is best accomplished by means of the  $(c, T)$  phase diagram (Figures 1, 2). We focus on the  $c = 0$  side of the diagram. The intriguing aspect of this phase diagram is that liquid and solid are not separated by a single curve, but by two curves (called liquidus and solidus), which merge at the melting

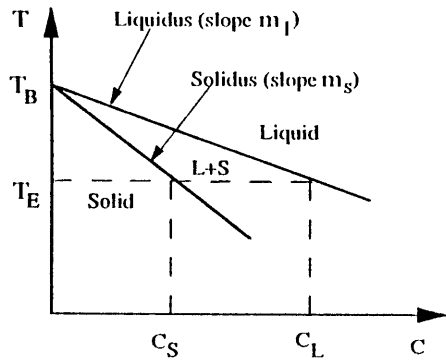


Fig. 1a

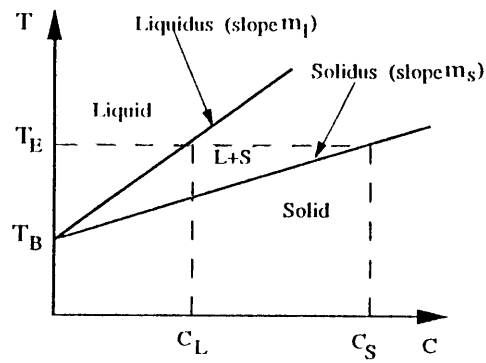


Fig. 1b

Fig. 1. Idealized phase diagrams in the neighborhood of  $(c, T) = (0, T_B)$  which display linear liquidus and solidus lines which separate the single phase regions from the coexistence region. This idealization is inherent in typical sharp interface alloy models (one-phase or two-phase) and represents a local approximation to the phase diagram displayed in Figure 2. Figure 1a assumes negative slopes for the liquidus and solidus lines while Figure 1b assumes they are positive. The sign of the slopes determines which phase has higher solute concentration. In Figure 1a, solute from the liquid must be rejected as the material freezes. The phase-field-alloy model we discuss is not restricted to constant slopes, but asymptotically approaches constant slopes in the neighborhood of small  $c$ .

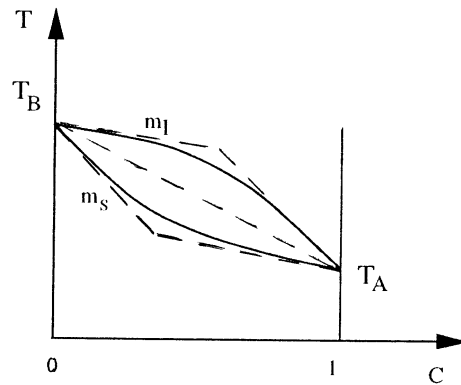


Fig. 2. The phase diagram for the range of  $c$  values displaying the melting temperatures  $T_A$  and  $T_B$  for the pure materials  $A$  and  $B$ . The liquidus is given by the upper curve while the solidus is given by the lower curve. The extent to which the liquidus and solidus are separated from the line connecting  $(0, T_B)$  and  $(1, T_A)$  is determined by the physical parameters. The phase diagram can be obtained from the free energy through the phase field alloy model (in equilibrium) so that the liquidus is  $c^+(T)$  and the solidus is  $c^-(T)$ .

temperature  $T_B$  of the pure  $B$  material ( $c = 0$ ). To a reasonable approximation for small  $c$ , one may assume that these two curves are linear. To be specific, we discuss the phase diagram displayed in Figure 1a for the purpose of stating the simple traditional models. At a fixed temperature  $T_i < T_B$  the liquidus line intersects with  $T = T_i$  at a point  $c_L$  while the solidus intersects at  $c_S$ . Thus one expects an interface at equilibrium at temperature  $T_i$  to exhibit concentration  $c_S$  on the liquidus side and  $c_L$  on the solid. That is, the concentration is a piecewise constant function with a jump between  $c_L$  and  $c_S$  at the phase boundary.

While the (equilibrium) phase diagram explains (a), it is irrelevant to (b) since the latter describes a dynamical phenomenon, exhibited in the (concentration) diffusion equation below. The dynamical modelling of the alloy problem is typically accomplished by means of a (sharp-interface) free-boundary problem which often accounts for only the liquid phase ("one-phase problem") thereby neglecting the diffusion of impurities in the solid, which is so small. Also, the concentration of impurities is assumed to be so small that one does not need to regard the thermodynamic variables such as latent heat as functions of  $c$ .

*The Two-Phase (Sharp-Interface) Problem.* Thus, a reasonable two-phase description of the dilute binary alloy based on the discussion of the one-phase problem in [S2] and the two-phase problem in [O, Xi2] may be written as:

*The Two-Phase Alloy Model.* We consider the coupled system for  $(T, c, \Gamma)$  satisfying (1.1), (1.2) and

$$c_t = K_2^\pm \Delta c \quad \text{in } \Omega \setminus \Gamma(t), \quad (2.1)$$

$$-v[c]^\pm = [K_2 \nabla c \cdot n]^\pm \quad \text{on } \Gamma(t), \quad (2.2)$$

$$T - T_B = -\frac{\sigma}{[s]_E}(\kappa + \alpha v) + \frac{1}{2}(m_l c_+ + m_s c_-) \quad \text{on } \Gamma(t), \quad (2.3)$$

$$m_l c_+ = m_s c_- \quad (2.4)$$

where  $T_B$  is the melting temperature of the pure  $B$  material (i.e.,  $T_M$  in (1.4)) and  $c_+$  represents the limit of  $c$  from the liquid side (and  $c_-$  from the solid side), while  $[\cdot]^\pm$  is the difference between the limits from the liquid and solid sides. Also,  $K_2^\pm$  are the diffusivities of the solute in the liquid and solid phases, respectively, and all other parameters are as defined in Section 1.

We note that the last term in (2.3) has been written to reflect the symmetry of the situation since clearly (in equilibrium) we have  $m_l c_+ = m_s c_-$  ( $c_+ = c_L$ ,  $c_- = c_S$  in equilibrium). In fact, equation (2.3), which is a generalization of the interface relation (1.4), can be understood very simply in terms of the basic phase diagram (Figure 1). If we consider a stationary planar interface, then  $\kappa = v = 0$  in (2.3) so that the value of  $T$  is given by

$$T - T_B = \frac{1}{2}(m_l c_+ + m_s c_-) = m_l c_L = m_s c_S. \quad (2.5)$$

This means that the temperature  $T$  is compatible with the coexistence of liquid and solid phases if the liquid has concentration  $c_L$  and the solid  $c_S$ , as shown by the horizontal line in Figures 1a or 1b. Thus, (2.3) represents a modification of (1.3) in

which the equilibrium alloy effects are combined linearly with the Gibbs-Thomson (namely, the  $\sigma\kappa$  term) and the kinetic undercooling ( $\alpha\sigma v$  term) effects.

*The One-Phase (Sharp-Interface) Problem.* The single-phase version of (2.1)–(2.4) is obtained by suppressing the role of concentration in the solid while maintaining some of the key relationships in the phase diagram. In particular, the relation (2.3) is replaced by the single-phase version

$$T - T_B = -\frac{\sigma}{[s]_E}(\kappa + \alpha v) + m_l c \quad \text{on } \Gamma(t) \quad (2.3')$$

where we can unambiguously write  $c$  (rather than  $c_+$  or  $c_-$ ) since we are only concerned with concentration in the liquid. Furthermore, by making the approximation that the jump  $[c]_{\pm}^{\pm}$  in  $c$  in the dynamics is equal to that of the statics, i.e.,  $[c]_{\pm}^{\pm} = c_L - c_S$ , and using the definition

$$j \equiv \frac{c_S}{c_L} \quad \text{or} \quad c_L - c_S = (1 - j)c_L \quad (2.5a, b)$$

we can write the analogue of (2.2) as

$$-(1 - j)v c = K_2^+ \nabla c \cdot n \quad \text{on } \Gamma(t) \quad (2.2')$$

where  $c$  again denotes concentration in the liquid (i.e.,  $c_+$  on the interface). The right-hand side of (2.2') has been further simplified by assuming that the limit of  $\nabla c$  on the interface from the solid side can be neglected. The rationale for this would be that the physical effects of diffusion and conservation of mass are adequately represented. In other words, equation (2.2') expresses the idea that the excess concentration which is deposited (or absorbed) at the interface as a result of different concentrations in the two phases must diffuse into the material in order to conserve mass. The modification of (2.2) to (2.2') implies the hope that allowing this excess to diffuse into the liquid alone does not change the physical picture drastically. Thus the issues involved in a "one-phase alloy" problem are similar to those in the "one-phase Stefan" problems, and the difficulties demonstrated in [O] are also similar. Nevertheless, our objective is not to endorse the "one-phase" approach but merely to demonstrate its relationship to the other models and mention that its use leads to some exact solutions and stability calculations. The problem is usually written as a system which is coupled to a two-phase temperature system but can easily be modified to render a system with truly one phase in both temperature and concentration.

*The One-Phase Alloy Model.* Consider a system for  $(T, c, \Gamma)$  satisfying (1.1), (1.2), (2.2'), (2.3') and

$$c_t = K_2^+ \Delta c \quad \text{in liquid.} \quad (2.1')$$

For the *completely* one-phase problem, consider (1.1) also to be valid in the liquid only, while (1.2) is modified to

$$\rho l v = K_1 \nabla T \cdot n \quad \text{on } \Gamma(t). \quad (1.2')$$

Thus the completely one-phase model involves a time-dependent domain, with part of the boundary consisting of  $\Gamma(t)$ .

In addition to the similarities between the one-phase alloy and one-phase Stefan models, there are some important differences. In terms of thermal diffusion, the differences between the two phases is usually not vast, so that neglecting one of the two phases is a mathematical convenience, and any degeneracies which may arise are mathematical artifacts. For the alloy problem, however, there is usually a large difference in the diffusivity of solute, i.e.,  $K_2^- \ll K_2^+$ , and  $K_2^-$  is generally close to zero. Thus, at least part of the degeneracy, embodied in (2.1) as  $K_2^-$  vanishes, is generic to the physical problem, and presents a fundamental issue which is independent of the particular mathematical approach.

## 2.2. A Thermal-Alloy Phase Field Model

We consider a model, based on the phase-field ideas of Section 1, which incorporates the physics of binary alloys in addition to thermal properties. Our aim here is to study the simplest set of equations which with (a) exhibit the proper behavior as the interface thickness  $\varepsilon$  approaches zero, and (b) identify all of the material parameters (see Figure 3).

We begin by considering a free energy  $\mathcal{F}$ , which describes the intermediate phase and concentration,

$$\begin{aligned} \mathcal{F}(\phi, c, T) = \int d^N x \left\{ \frac{\xi_A^2}{2} (\nabla\phi)^2 c + \frac{\xi_B^2}{2} (\nabla\phi)^2 (1-c) + \frac{1}{8a_A} (\phi^2 - 1)^2 c \right. \\ \left. + \frac{1}{8a_B} (1-c)(\phi^2 - 1)^2 - \frac{[s]_A}{2} (T - T_A)\phi c \right. \\ \left. - \frac{[s]_B}{2} (T - T_B)\phi(1-c) + Vc(1-c) \right. \\ \left. + RT\{c \ln c + (1-c) \ln(1-c)\} - C_V T \ln T \right\}. \end{aligned} \quad (2.6)$$

Here, the subscripts  $A$  and  $B$  denote the two materials, respectively. Briefly, the free energy is constructed by considering the analogous terms for each of the pure materials. For each term we assume a linear crossover between the two terms. For the sake of simplicity, we have omitted the temperature dependence in the  $\xi_{A,B}$  and  $a_{A,B}$  terms [CJ] which would provide additional nonlinear temperature terms.

The free energy can be interpreted geometrically in a four-dimensional space  $(\phi, c, T, \mathcal{F})$ . For the pure phases,  $\phi = \pm 1$ ; the free energy is experimentally well established for all concentrations. For the pure materials,  $c = 0, 1$ , we have (for the entire range of  $\phi$ ) the usual phase-field equations for a pure material. Thus, mathematical modelling of the free energy entails assigning values for  $\mathcal{F}$  in the intermediate regions  $|\phi| < 1$ , representing the four-dimensional space within the more established three-dimensional hyperplanes.

The first two terms involve the gradient of  $\phi$  terms, which arise from the microscopic interaction strengths. The coefficients  $\xi_A$  and  $\xi_B$  are characteristics of the

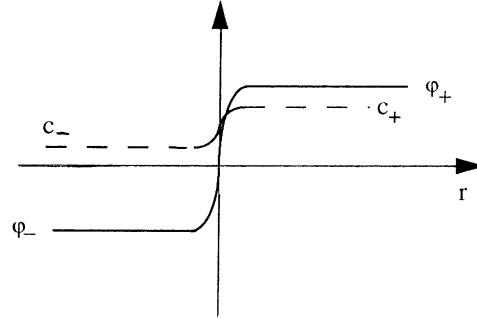


Fig. 3. Profiles of  $\phi$  and  $c$  across the interface. In phase-field models, a phase change corresponds to a transition layer in the order parameter,  $\phi$ , while temperature  $T$  has a transition layer in its gradient, the concentration  $c$  has a transition layer which is similar to that of  $\phi$ . However, while  $\phi$  always has a transition from (approximately)  $-1$  to  $1$ , the transition in  $c$  (between the two positive values  $c_S$  and  $c_L$ ) depends on the temperature, in accordance with the phase diagram of Figure 2.

two materials, as are the ‘well depths’ of the double-well potentials, denoted  $a_A$  and  $a_B$ . The third and fourth terms are thus linear combinations of the analogous terms for the homogeneous materials. The next two terms involve the entropy differences between the two phases for the pure materials, denoted  $[s]_A$  and  $[s]_B$ . The temperatures  $T_A$  and  $T_B$  are the equilibrium melting temperatures of the two materials. The quadratic term in  $c$  arises from the differences in the bonding energies between the  $A$  atoms and the  $B$  atoms [Co], so that  $V$  is an energy density. The terms containing the logarithm of  $c$  constitute the entropy of mixing [Co]. The last term involves the specific heat  $C_V$  per unit volume. By setting  $c$  at 0 or 1, one has the free energy of the pure  $A$  or  $B$  material, respectively.

We write three equations describing  $(\phi, c, T)$ . The concentration  $c$  satisfies a conserved variational formulation

$$\tau_1 c_t = \nabla \cdot K_2(\phi, c)c(1-c)\nabla \frac{\delta F}{\delta c}, \quad (2.7)$$

while the usual phase field (nonconserved) applies to  $\phi$ ,

$$\tau_2 \phi_t = -\frac{\delta F}{\delta \phi}. \quad (2.8)$$

Here,  $\tau_1$  and  $\tau_2$  are relaxation constants while  $K_2(\phi, c)c(1-c)$  is the mobility term. In general,  $K_2$  may depend on phase and concentration, but usually varies most significantly as phase changes. The term  $c(1-c)$ , also used by [WBM1], is a standard approximation reflecting the fact that mobility vanishes in the two phases and attains a peak at equal concentrations of the two materials. The energy conservation equation arises [CJ] from thermodynamic balance equations as

$$C_V T_t + \frac{1}{2} \left( l(c)\phi_t - (Q + [l]_{B,A}\phi)c_t \right) = \nabla \cdot K_1 \nabla T, \quad (2.9)$$

where

$$l(c) \equiv (T_A[s]_A c + T_B[s]_B(1-c)), \quad (2.10)$$

$$[l]_{B,A} \equiv (T_B[s]_B - T_A[s]_A), \quad (2.11)$$

$$Q \equiv 2(T_B - T_A) \left( C_V + \frac{s^l + s^s}{2} \right), \quad (2.12)$$

and  $C_V$  and  $K_1$  are the specific heat and the thermal conductivity.

Note that  $l(c)$  is the analogue of the usual latent heat since a basic thermodynamic relation implies that latent heat of the pure  $A$  material is  $T[s]_A$ . In the limit of a pure material, equation (2.9) clearly reduces to the usual heat equation.

Similarly, the concentration equation (2.7) may be written as

$$\tau_1 c_t = \nabla \cdot K_2(\phi, c) c(1-c) \nabla \Sigma_i \frac{\partial f_i}{\partial c}, \quad (2.13)$$

where

$$\frac{\partial f_1}{\partial c} \equiv (\xi_A^2 - \xi_B^2)(\nabla \phi)^2, \quad (2.14)$$

$$\frac{\partial f_2}{\partial c} \equiv \frac{1}{8}(\phi^2 - 1) \left( \frac{1}{a_A} - \frac{1}{a_B} \right), \quad (2.15)$$

$$\frac{\partial f_3}{\partial c} \equiv V - 2Vc, \quad (2.16)$$

$$\frac{\partial f_4}{\partial c} \equiv \frac{1}{2} \left\{ -[s]_A(T - T_A) + [s]_B(T - T_B) \right\} \phi, \quad (2.17)$$

$$\frac{\partial f_5}{\partial c} \equiv RT \ln \frac{c}{1-c}. \quad (2.18)$$

The relative importance of these terms will be discussed below in this section. The phase equation (2.8) can be written as

$$\frac{2\varepsilon}{3\sigma} \tau_2 \phi_t = \varepsilon^2 \Delta \phi + \frac{1}{2}(\phi - \phi^3) + \frac{2\varepsilon}{3\sigma} \left\{ [s]_A(T - T_A)c + [s]_B(T - T_B)(1-c) \right\}, \quad (2.19)$$

where

$$\sigma(c) \equiv \frac{2}{3} \left\{ \xi_A^2 c + \xi_B^2(1-c) \right\}^{1/2} \left\{ \frac{c}{a_A} + \frac{1-c}{a_B} \right\}^{1/2}, \quad (2.20)$$

$$\varepsilon(c) \equiv \left\{ \xi_A^2 c + \xi_B^2(1-c) \right\}^{1/2} \left\{ \frac{c}{a_A} + \frac{1-c}{a_B} \right\}^{-1/2}. \quad (2.21)$$

This equation differs from the pure version in that the entropy term is a linear combination of the entropy terms for each of the pure materials, and  $\varepsilon$  and  $\sigma$  both depend on  $c$ .

Hence, equations (2.19), (2.9), and (2.13) are a system to be studied subject to appropriate initial and boundary conditions. Note that if the total mass of each material is constant, then Neumann conditions for concentration are appropriate, and the equation (2.13) is in full conservation form. The boundary conditions for temperature are imposed in accordance with the thermal environment, e.g., Dirichlet conditions if the alloy is in a container whose walls remain at constant temperature, or Neumann conditions if it is insulated.

### 2.3. Basic Components of Equations

We first discuss the various aspects of the three equations with the aim of isolating those terms which are crucial to the behavior of a sharp interface. Equation (2.19) has a form similar to the pure version in that a transition layer is induced in the limit as  $\varepsilon(c)$  approaches zero. Although different limits may be considered, we are primarily interested in the limit in which the interface thickness approaches zero while surface tension remains finite. The surface tension is more complicated for the alloy as discussed in Section 3. Thus, we consider the limit of  $\xi_A, \xi_B, a_A,$  and  $a_B$  approaching zero with  $\xi_A/\xi_B, a_A/a_B$  and  $\sigma(c)$  held fixed (for fixed  $c$ ), while  $\varepsilon(c)$  approaches zero (for fixed  $c$ ). Since we use  $\varepsilon(c)$  as a free parameter, with the ansatz that the width of the interface is not as significant physically as the other parameters such as surface tension and entropy, we replace the coefficient of  $\Delta\phi$  (in the simplest case), by a parameter  $\varepsilon^2$  which is independent of  $c$  in the asymptotic calculations. A minimum set of criteria for the concentration equation to be physically reasonable has the following limiting properties:

- (1) In the limit  $\varepsilon \rightarrow 0$ , the solution  $c$  must satisfy the diffusion equation in each of the pure phases.
- (2) A transition layer near the interface must be induced on  $c$  for small  $\varepsilon$ .
- (3) Appropriate interface conditions must be attained in the limit  $\varepsilon \rightarrow 0$  so that the jump in  $c$  balances the jump in the derivative of  $c$ , thereby ensuring the conservation of mass.

If  $K_2$  is asymptotically small in the solid phase (e.g., of order  $O(\varepsilon)$ ), then the equation must have the property:

- (4) In the limit  $\varepsilon \rightarrow 0$ , the concentration satisfies the diffusion equation in the liquid, and  $c_t = 0$  in the solid.

It is clear that the concentration-diffusion equation arises from the entropy of mixing term,  $\partial f_5/\partial c = RT \ln\{c(1 - c)^{-1}\}$ . Mathematically, this follows from (2.13) and (2.18) yielding

$$\begin{aligned} \tau_1 c_t &= \nabla \cdot K_2(\phi, c)c(1 - c)\nabla RT \ln \frac{c}{1 - c} \\ &= \nabla \cdot K_2(\phi, c)\left[RT\nabla c + R\nabla Tc(1 - c) \ln \frac{c}{1 - c}\right], \end{aligned} \tag{2.22}$$

where the last term is small unless both the thermal gradient and concentration are both substantial. In the limit of a sharp interface one expects (in general) a discontinuity in  $c$ , even in equilibrium. The chief mechanism for forcing this transition

layer is the term  $\partial f_4/\partial c$  in (2.17), which has the form  $(M_1 + M_2 T)\phi$  where  $M_1$  and  $M_2$  are constants. Since  $T$  is not expected to have a transition-layer behavior, one may examine the term  $M_1\phi$  in order to understand the qualitative behavior. Thus, if we write (2.13) by omitting all terms but the entropy of mixing term  $\partial f_5/\partial c$ , and the entropy of phase term  $\partial f_4/\partial c$ , then we have the *fundamental concentration equation*

$$\begin{aligned} c_t &= \nabla \cdot K_2(\phi, c)c(1-c)\nabla \left\{ \ln \frac{c}{1-c} + M\phi \right\} \\ &= \nabla \cdot \left\{ K_2(\phi, c) \left( \nabla c + Mc(1-c)\nabla\phi \right) \right\}. \end{aligned} \quad (2.23)$$

For small  $c$ , we can consider in one-dimensional space its simplification

$$c_t = \frac{\partial}{\partial x} \left\{ K_2(\phi, c) \left( c_x + Mc\phi_x \right) \right\}. \quad (2.24)$$

Here, we have suppressed all constants except  $M$ , which we retain since this coefficient may have either sign depending on the constants in  $\partial f_4/\partial c$ . In general one expects  $K_2(1, c) \neq K_2(-1, c)$  since the solid and liquid have very different diffusion constants. However, it is evident from (2.23) that a transition layer in  $\phi$  forces a transition layer in  $c$  even if  $K_2 = 1$  and time dependence is neglected, since in that case  $c = Be^{-M\phi}$ . On the other hand, if

$$K_2(\phi, c) = \frac{1}{2}(k_l - k_s)(\phi + 1) + k_s, \quad (2.25)$$

where  $k_l$  and  $k_s$  are the diffusion constants for liquid and solid, respectively, so that  $K_2$  has a transition layer of small width,  $\varepsilon$ ; then one has a more complicated asymptotics but a similar transition layer for  $c$ . If, for example,  $k_s = \varepsilon$ , then a transition layer can occur even without the  $M\phi$  term but the transition layer then disappears after a very long time. This aspect of the fundamental concentration equation can be illuminated in an analogy with heat diffusion: Whenever  $M = 0$ , one can view equation (2.23) as a heat equation with  $c$  defined as temperature. If, in addition,  $K_2$  is given by (2.25) with  $\phi$  defined to be a function with a transition layer at  $x = 0$ , e.g.,  $\phi(x) = \tanh(x/\varepsilon)$ , then (2.23) can be regarded as a heat equation describing a material which is a ‘fusion’ of highly thermally conductive material for  $x > \varepsilon$  (e.g., aluminium) and a thermally insulating material for  $x < -\varepsilon$  (e.g., asbestos). In the region  $|x| \leq \varepsilon$ ,  $K_2$  makes a transition between  $\varepsilon$  and 1.

We consider this material in a finite one-dimensional strip subject to boundary conditions  $c_x = 0$  at both ends and smooth initial conditions in a bell-shaped curve (without a transition layer). Under these conditions the evolution of (2.23) soon leads to a transition layer, since the rapid diffusion on the right side leads to a drop in temperature near the center-right, while the left side remains relatively unchanged. Since the solution to this evolution equation must be smooth (for any finite  $\varepsilon$ ), the formation of a smooth transition layer is the result. However, the transition layer must eventually disappear since the time-independent equation has only constant solutions. We demonstrate this asymptotically in Section 3 and prove it rigorously in Section 5.

The transition layer just described has both similarities and differences with that of (2.23) with  $K_2 = 1$ , which supports layers in equilibrium.

Examining the other terms in (2.13) we note that  $\partial f_3/\partial c = V(1-2c)$  arises from the possible difference in the interaction potential between unlike atoms compared with like atoms. Thus, for an ‘ideal solution’ one has  $V = 0$  and this term is neglected. We also note that for dilute solutions, i.e., for small  $c$ , this term is  $O(c^2)$  in (2.13) in comparison with the  $O(c)$  term generated by  $\partial f_5/\partial c$ .

The terms  $\partial f_1/\partial c$  and  $\partial f_2/\partial c$  arise from the differences in the microscopic constants  $\xi_A, \xi_B$  and  $a_A, a_B$ . These terms are less significant and may be neglected in a basic analysis due to the following observations:

(1) From a purely macroscopic perspective one can set  $\xi_A = \xi_B$  and  $a_A = a_B$ , while  $[s]_A \neq [s]_B$ . Since the macroscopic limits involve the capillarity length  $d_0$ , which is entropy divided by surface tension, one can obtain the correct capillarity length by adjusting only  $[s]_A$  and  $[s]_B$ .

(2) In the asymptotic analysis, these terms do not contribute to the limiting equations (in both solid and liquid phases). The details of these calculations are presented in Section 3.

The heat equation (2.9) consists of: (1) the terms involving  $C_V$  and  $K_1$ , which are common to the pure material in a single phase (of course,  $C_V$  and  $K_1$  may depend on both  $c$  and  $\phi$ ), (2) the term involving  $\phi_t$ , which is the generalization of the latent heat, part of which is just a linear interpolation between the latent heats of the two materials  $T[s]_A$  and  $T[s]_B$  [CJ]. The term involving  $[l]_{B,A}$  accounts for the changes in heat due to the entropy differences in the materials.

### 3. Asymptotic Analysis

We summarize some of the conclusions that can be obtained from a formal asymptotic analysis, using methods that are similar to those of CAGINALP & XIE [CX1,2]. The thermal alloy phase-field model of Section 2 can be written as:

$$\alpha \varepsilon^2 E(c) \phi_t = \varepsilon^2 E(c) \Delta \phi + \frac{1}{2} (\phi - \phi^3) + \frac{\varepsilon}{3\sigma(c)} \left\{ [s]_A (T - T_A) c + [s]_B (T - T_B) (1 - c) \right\}, \quad (3.1)$$

$$C_V T_t + \frac{1}{2} \left( l(c) \phi_t - (Q + [l]_{B,A} \phi) c_t \right) = \nabla \cdot K_1 \nabla T, \quad (3.2)$$

$$c_t = \nabla \cdot K_2(\phi) c (1 - c) \nabla \left[ (M + M_1 T) \phi + RT \ln \frac{c}{1 - c} \right] \quad (3.3)$$

with

$$\begin{aligned} \varepsilon^2(c) &= \left\{ \xi_A^2 c + \xi_B^2 (1 - c) \right\} \left( \frac{c}{a_A} + \frac{1 - c}{a_B} \right)^{-1} \\ &= \xi_B^2 a_B \frac{1 - c + (\xi_A^2/\xi_B^2)c}{1 - c + (a_B/a_A)c} = \xi_A^2 a_A \frac{c + (\xi_B^2/\xi_A^2)(1 - c)}{c + (a_A/a_B)(1 - c)}, \end{aligned} \quad (3.4)$$

$$a(c) = \left( \frac{c}{a_A} + \frac{1-c}{a_B} \right)^{-1} = \frac{a_B}{1-c + (a_B/a_A)c} = \frac{a_A}{c + (a_A/a_B)(1-c)} \quad (3.5)$$

where  $E(c) = \varepsilon^2(c)/\varepsilon^2$  and  $\sigma(c)$  are two bounded functions with positive lower bound,  $\varepsilon$  in (3.1) is a (small) positive constant and the other constants are defined in Section 2. We can then verify

**Proposition 3.1.** *In the limit as  $\varepsilon \rightarrow 0$ , the first-order approximation  $(\phi^0, T^0, c^0)$  of the solution  $(\phi, T, c)$  to (3.1)–(3.3) is governed by the sharp-interface model:*

$$\begin{aligned} C_V T_t^0 - \frac{1}{2} (Q \pm [l]_{B,A}) c_t^0 &= K_1 \Delta T^0 \quad \text{in } \Omega \setminus \Gamma(t), \\ c_t^0 = \nabla \cdot K_2^\pm c^0 (1 - c^0) \nabla [RT^0 \ln \frac{c^0}{1-c^0} \pm M_1 T^0] &\quad \text{in } \Omega \setminus \Gamma(t), \end{aligned} \quad (3.6)$$

and on the interface  $\Gamma(t)$

$$\begin{aligned} [T^0]^\pm &= 0, \\ [K_1 T_r^0]^\pm &= \frac{1}{2} (Q[c^0]^\pm + [l]_{B,A}(c_+^0 + c_-^0) - 2T_B[s]_B) v^0, \\ RT^0 [\ln \frac{c^0}{1-c^0}]^\pm &= -2(M + M_1 T^0), \\ [K_2 RT^0 c_r^0]^\pm + [RK_2 c^0 (1 - c^0) (\ln \frac{c^0}{1-c^0}) T_r^0]^\pm & \\ + K_2^+ M_1 c_+^0 (1 - c_+^0) (T_r^0)_+ + K_2^- M_1 c_-^0 (1 - c_-^0) (T_r^0)_- &= -[c^0]^\pm v^0 \end{aligned} \quad (3.7)$$

subject to a Gibbs-Thomson-type relation on  $\Gamma(t)$ :

$$\int_{R^1} (H_1 + H_2) \psi(z) dz = 0 \quad (3.8)$$

where  $H_1, H_2$  are given by

$$\begin{aligned} H_1 &\equiv (\alpha v^0 + \kappa^0) \hat{\phi}_z^0 + \frac{1}{3E(\hat{c}^0)\sigma(\hat{c}^0)} (a + b\hat{c}^0), \\ H_2 &\equiv \frac{E'(\hat{c}^0) \hat{\phi}_{zz}^0}{\bar{R}E(\hat{c}^0)} \hat{c}^0 (1 - \hat{c}^0) \left[ -v^0 \int_0^z \frac{dy}{K_2(\hat{\phi}^0)(1 - \hat{c}^0)} \right. \\ &\quad \left. + c_4(s, t) \int_0^z \frac{dy}{K_2(\hat{\phi}^0)\hat{c}^0(1 - \hat{c}^0)} + c_6(s, t) \right] \end{aligned} \quad (3.9)$$

and  $\psi = \hat{\phi}_z^0$ , where  $\hat{\phi}^0$  is a solution of the system

$$\begin{aligned} E(\hat{c}^0) \hat{\phi}_{zz}^0 + \frac{1}{2} (\hat{\phi}^0 - (\hat{\phi}^0)^3) &= 0, \\ \left\{ K_2(\hat{\phi}^0) \hat{c}^0 (1 - \hat{c}^0) \left( \bar{A} \hat{\phi}^0 + \bar{R} \ln \frac{\hat{c}^0}{1 - \hat{c}^0} \right) \right\}_z &= 0, \\ \hat{\phi}^0(-\infty) = -1, \quad \hat{\phi}^0(0) = 0, \quad \hat{\phi}^0(\infty) = 1, \\ \hat{c}^0(-\infty) = c_-^0, \quad \hat{c}^0(\infty) = c_+^0. \end{aligned} \quad (3.10)$$

$\bar{A} = M + M_1 \hat{T}^0$ ,  $\bar{R} = R \hat{T}^0$ ,  $c_4(s, t)$  and  $c_6(s, t)$  are constants independent of  $z$ , and  $a + bc \equiv [s]_A(\hat{T}^0 - T_A)c + [s]_B(\hat{T}^0 - T_B)(1 - c)$ . (Detailed discussion for the system (3.10) is presented in [CX2].)

In particular, if  $E(c) = 1$ , then the system (3.10) can be solved explicitly and the integral in (3.8) can be evaluated. This leads to the interface condition on  $\Gamma(t)$ :

$$\begin{aligned} \alpha v^0 + \kappa^0 = & \frac{RT^0}{2(M + M_1 T^0)} \left[ [s]_A(T^0 - T_A) \int_{c_-^0}^{c_+^0} \frac{du}{\sigma(u)(1 - u)} \right. \\ & \left. + [s]_B(T^0 - T_B) \int_{c_-^0}^{c_+^0} \frac{du}{\sigma(u)u} \right]. \end{aligned} \tag{3.11}$$

#### 4. Interaction Between Dynamic and Static Transition Layers

We now compare two equations, one having only a dynamic transition layer, and the other having both dynamic and static layers:

$$u_t = \frac{\partial}{\partial x} \left\{ D(\phi^\varepsilon) u_x \right\}, \tag{4.1}$$

$$c_t = \frac{\partial}{\partial x} \left\{ D(\phi^\varepsilon) (c_x + Ac(1 - c)\phi_x^\varepsilon) \right\}, \tag{4.2}$$

with appropriate boundary and initial conditions, where

$$\phi^\varepsilon(x) \equiv \tanh \frac{x}{\varepsilon}, \quad \varepsilon > 0. \tag{4.3}$$

The first equation is just the heat equation, with a variable diffusion coefficient  $D$ , exhibiting a transition layer near  $x = 0$ . In particular, we can imagine a thin rod consisting of two materials, with very different heat conduction properties, fused together at  $x = 0$ . The second is just the simplest concentration equation with a change of phase at  $x = 0$ . This means that thermal conditions are balanced so that the interface remains fixed.

We consider the cases

$$(i) \quad D(\phi^\varepsilon) = \frac{1}{2}(3 + \phi^\varepsilon), \tag{4.4}$$

$$(ii) \quad D(\phi^\varepsilon) = \frac{1}{2}(1 + \phi^\varepsilon). \tag{4.5}$$

In particular, the form of  $D$  expressed by (4.5) involves a degeneracy in that  $D$  approaches zero as  $x$  approaches  $-\infty$ . In each of these equations, a transition layer arises in  $u$  and  $c$ , even if the initial conditions do not involve a steep gradient (i.e., one of order  $1/\varepsilon$ ). In equation (4.2) a transition layer in  $c$  occurs even if  $D = 1$ , according to the formal asymptotic of Section 3. One of our goals is to obtain a rigorous understanding of the similarities and differences in the transition layers which arise from various physical effects, particularly, the following three situations:

- (A) Equation (4.2) with  $A = 0$  (namely, equation (4.1)) subject to (4.4) or (4.5).
- (B) Equation (4.2) with  $D = 1$ .
- (C) Equation (4.2) subject to (4.4) or (4.5).

The transition layer which arises in (A) is a consequence of the change in the diffusion coefficient. The physical origin of this is in the differences of heat diffusion in the two materials (in (4.1)) or of mass diffusion in the two phases. This is clearly a dynamical effect and the transition layer forms and then disappears in finite time. On the other hand the transition layer in (B) occurs even in equilibrium and has no analog for thermal diffusion. It arises from the particular nature of the phase diagram (Figure 3) in which the liquidus and solidus are separated by a finite distance at a fixed temperature ( $|c_l - c_s|$ ), which is in fact the size of the jump in (4.2) as  $t \rightarrow \infty$ . The transition layer in (C) combines both of these effects and permits the study of the interaction between the development and disappearance of the diffusion-induced layer with the evolution of the phase diagram layer.

(1a) We first consider the simpler case in which  $D(\phi^\varepsilon)$  is given by (4.4), which avoids the degeneracy problem. The precise problem which we consider here is

$$\begin{aligned}
 u_t &= \frac{\partial}{\partial x} \left\{ D(\phi^\varepsilon) u_x \right\}, & x \in (-1, 1), \quad t > 0, \\
 u_x(-1, t) &= u_x(1, t) = 0, & t > 0, \\
 u(x, 0) &= u_0(x), & -1 < x < 1,
 \end{aligned}
 \tag{4.6}$$

where  $u_0(x)$  is a given function (e.g.,  $u_0(x)$  is continuous on the interval  $(-1, 1)$ ).

For any  $\varepsilon > 0$ , the problem (4.6) possesses a unique solution  $u^\varepsilon(x, t)$ , which is smooth in  $Q_T \equiv (-1, 1) \times (0, T)$ , and  $u^\varepsilon \in C^{2,1}(\overline{Q_T})$  if we assume that  $u_0(x) \in C^2[-1, 1]$  and the consistency condition  $u'_0(\pm 1) = 0$ . We investigate the behavior of  $u^\varepsilon(x, t)$  as  $\varepsilon \rightarrow 0^+$ .

Note first that the maximum principle gives the  $L^\infty$ -estimate

$$\|u^\varepsilon(x, t)\|_{L^\infty(Q_T)} \leq \|u_0(x)\|_{L^\infty(-1,1)},
 \tag{4.7}$$

and the energy estimate yields

$$\sup_{t \leq T} \int_{-1}^1 \left( u^\varepsilon(x, t) \right)^2 dx + 2 \int \int_{Q_T} D(\phi^\varepsilon) \left( u_x^\varepsilon \right)^2 dx dt \leq \int_{-1}^1 u_0^2(x) dx.
 \tag{4.8}$$

Then by the Ascoli-Arzelà compactness theorem, there exists a limit function  $u(x, t)$  such that, at least for a subsequence,

$$\begin{aligned}
 u^\varepsilon(x, t) &\rightarrow u(x, t) && \text{uniformly in } Q_T, \\
 u_x^\varepsilon(x, t) &\rightarrow u_x(x, t) && \text{in } L^2(Q_T).
 \end{aligned}$$

To identify the limit function  $u(x, t)$ , we note that  $u^\varepsilon(x, t)$  satisfies

$$\int \int_{Q_T} \left( -u^\varepsilon \zeta_t + D(\phi^\varepsilon) u_x^\varepsilon \zeta_x \right) dx dt = \int_{-1}^1 u_0(x) \zeta(x, 0) dx
 \tag{4.9}$$

for any smooth function  $\zeta(x, t) \in C^\infty(\overline{Q_T})$  with  $\zeta(\cdot, T) = 0$ . Since

$$\iint_{Q_T} D(\phi^\varepsilon) u_x^\varepsilon \zeta_x \, dx \, dt = \int_0^T \left( \int_{-1}^{-\varepsilon|\ln \varepsilon|} + \int_{-\varepsilon|\ln \varepsilon|}^{\varepsilon|\ln \varepsilon|} + \int_{\varepsilon|\ln \varepsilon|}^1 \right) D(\phi^\varepsilon) u_x^\varepsilon \zeta_x \, dx \, dt$$

and, by estimate (4.8),

$$\int_0^T \int_{-\varepsilon|\ln \varepsilon|}^{\varepsilon|\ln \varepsilon|} D(\phi^\varepsilon) u_x^\varepsilon \zeta_x \, dx \, dt \rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0^+.$$

Taking the limit  $\varepsilon \rightarrow 0^+$  in (4.9), we see that the function  $u(x, t)$  satisfies

$$\iint_{Q_T} -u \zeta_t + \int_0^T \left( \int_{-1}^0 u_x \zeta_x \, dx + \int_0^1 2u_x \zeta_x \, dx \right) dt = \int_{-1}^1 u_0(x) \zeta(x, 0) \, dx, \tag{4.10}$$

for any smooth function  $\zeta(x, t) \in C^\infty(\overline{Q_T})$  with  $\zeta(\cdot, T) = 0$ . By the regularity properties, we can show that the function  $u(x, t)$  satisfies

$$\begin{aligned} u_t &= u_{xx} & \text{if } -1 < x < 0, \quad t > 0, \\ u_t &= 2u_{xx} & \text{if } 0 < x < 1, \quad t > 0, \\ u(x, 0) &= u_0(x) & \text{in } -1 < x < 1, \\ u_x(-1, t) &= u_x(1, t) = 0 & \text{as } t > 0, \end{aligned} \tag{4.11}$$

and on the interface  $x = 0$ , we have

$$u^- = u^+, \quad u_x^- = 2u_x^+. \tag{4.12}$$

Note that the solution of the problem (4.11), (4.12) is unique, so that the whole sequence  $u^\varepsilon(x, t)$  (not just a subsequence) converges to  $u(x, t)$  uniformly.

To summarize, we have

**Theorem 4.1.** *Let  $u_0(x) \in C^2[-1, 1]$  satisfy the consistency conditions  $u_{0x}(\pm 1) = 0$  and let the function  $D(\phi^\varepsilon)$  be given by (4.4). Then the problem (4.6) possesses a unique solution  $u^\varepsilon(x, t)$  for any  $\varepsilon > 0$ . Moreover, the solution  $u^\varepsilon(x, t)$  converges to a function  $u(x, t)$  as  $\varepsilon \rightarrow 0$ , and the limit function  $u(x, t)$  is a unique solution to the problem (4.11) with interface conditions (4.12).*

Hence, we have proved that the diffused-interface problem (4.1), (4.4) has solutions which are governed to leading order by the sharp-interface problem (4.11) and (4.12). In physical terms, the problem in which two materials (with different diffusion coefficients) are joined together with a sharp boundary has a temperature distribution which is close to the problem in which the two materials are fused together over a distance  $\varepsilon$ .

(1b) Again, we assume that  $D(\phi^\varepsilon)$  is given by (4.4) and consider the problem

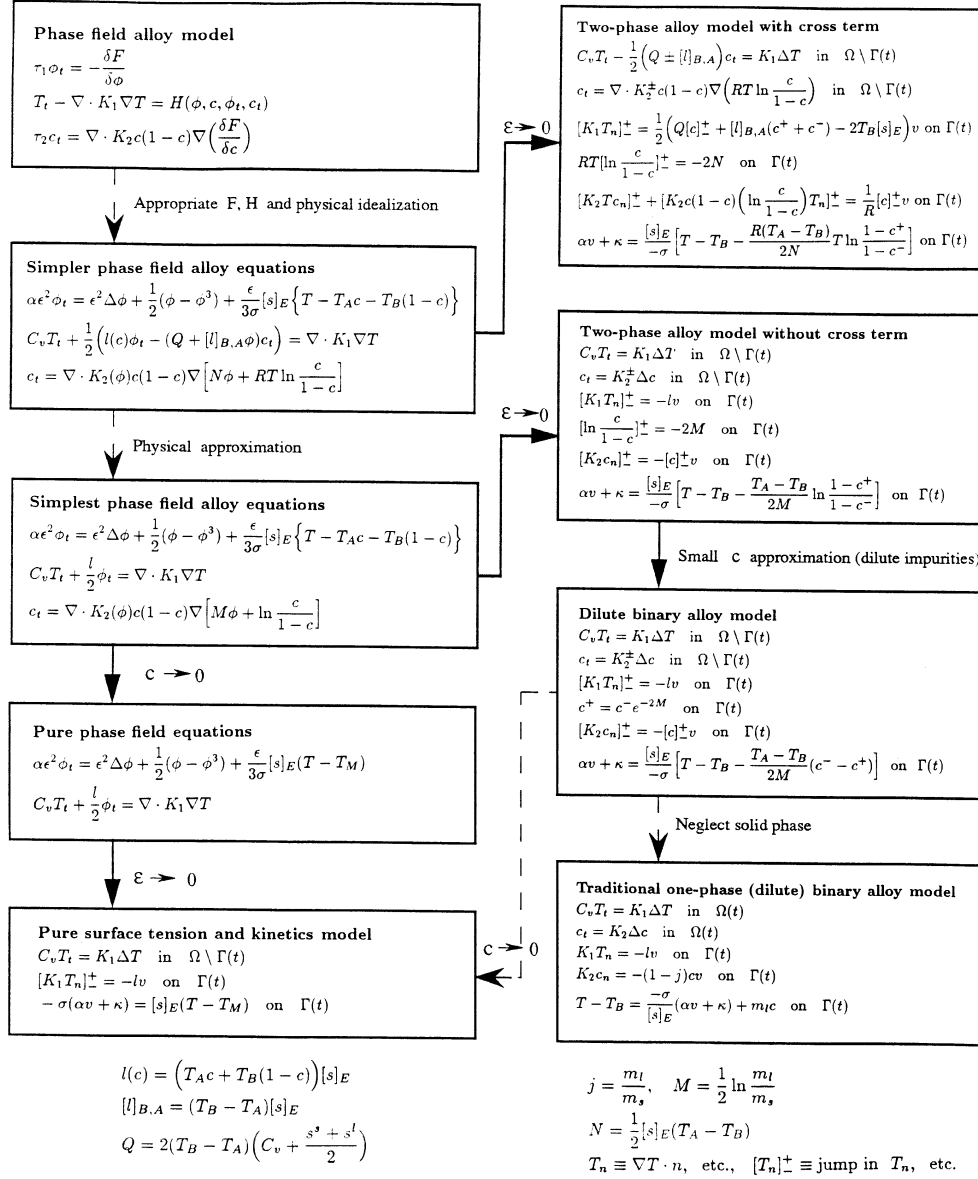


Fig. 4. Relationship between different alloy models. The most general phase-field model (upper left box) leads to a number of different limiting sets of equations, some of which are classical, e.g., the traditional one-phase (dilute binary alloy), and some are introduced in this paper, e.g., the two-phase alloy model without cross terms, in which the conditions involving  $c^+$  and  $c^-$  (not the derivatives of  $c$ ) are the new interface relations replacing the Gibbs-Thomson condition. With various simplifications and idealization, we obtain the "simplest" phase-field-alloy model which retains the key characteristics of an alloy. These idealizations consists of fixing, for example, the surface tension  $\sigma$ , for the mixture, which is accurate for pairs of materials with similar surface tension between phases, or for small concentrations of one material in another. The solid lines and arrows between the boxes indicate a mathematical relationship in the sense of a theorem for simpler geometries and matched asymptotic for more complicated geometries. The dashed lines indicate physical idealizations or approximations.

$$\begin{aligned}
c_t &= \frac{\partial}{\partial x} \left\{ D(\phi^\varepsilon) \left( c_x + Ac(1-c)\phi_x^\varepsilon \right) \right\} \quad \text{in } -1 < x < 1, \quad t > 0, \\
c_x(-1, t) &= c_x(1, t) = 0, \\
c(x, 0) &= c_0(x),
\end{aligned} \tag{4.13}$$

where  $c_0(x)$  is a given function with  $0 < c_0(x) < 1$  on  $-1 \leq x \leq 1$ , and  $A$  is a constant.

Problem (4.13) describes the simplest possible concentration problem with a stationary interface. When  $A = 0$ , we are again back to problem (4.6). When  $A$  is nonzero, the factor  $\phi_x^\varepsilon$  induces (for a small value of the parameter  $\varepsilon$ ) a transition layer in concentration  $c$ , so that the constant  $A$  characterizes the amplitude of the jump in concentration.

For any  $\varepsilon > 0$ , the problem (4.13) is a standard parabolic boundary-value problem, so that there exists a unique solution  $c^\varepsilon(x, t)$  that is smooth in  $Q_T$ . To see the behavior of  $c^\varepsilon(x, t)$  as  $\varepsilon \rightarrow 0^+$ , we need to obtain some estimates for the solution  $c^\varepsilon(x, t)$ . First, by use of the comparison principle and the condition  $0 < c_0(x) < 1$ , we can prove that

$$0 < c^\varepsilon(x, t) < 1. \tag{4.14}$$

Noting that  $c^\varepsilon(x, t)$  satisfies

$$c_t^\varepsilon = \frac{\partial}{\partial x} \left\{ D(\phi^\varepsilon) c^\varepsilon (1 - c^\varepsilon) \frac{\partial}{\partial x} \left( \ln \frac{c^\varepsilon}{1 - c^\varepsilon} + A\phi^\varepsilon \right) \right\}, \tag{4.15}$$

we let

$$f(\phi, c) = A\phi + \ln \frac{c}{1 - c}, \tag{4.16}$$

$$F(\phi, c) = \int_0^c f(\phi, y) dy = A\phi c + c \ln c + (1 - c) \ln(1 - c). \tag{4.17}$$

Then

$$\int_0^T \int_{-1}^1 f(\phi^\varepsilon, c^\varepsilon) \frac{\partial c^\varepsilon}{\partial t} dx dt = \int_0^T \int_{-1}^1 \frac{\partial}{\partial t} F(\phi^\varepsilon, c^\varepsilon) dx dt = \int_{-1}^1 F(\phi^\varepsilon, c^\varepsilon) \Big|_{t=0}^{t=T} dx.$$

Thus the quantity  $\int_0^T \int_{-1}^1 f(\phi^\varepsilon, c^\varepsilon) c_t^\varepsilon dx dt$  is bounded and the bound is independent of  $\varepsilon$ . Since

$$\begin{aligned}
& \int_0^T \int_{-1}^1 \frac{\partial}{\partial x} \left\{ D(\phi^\varepsilon) c^\varepsilon (1 - c^\varepsilon) \frac{\partial}{\partial x} f(\phi^\varepsilon, c^\varepsilon) \right\} f(\phi^\varepsilon, c^\varepsilon) dx dt \\
&= \int_0^T D(\phi^\varepsilon) c^\varepsilon (1 - c^\varepsilon) f(\phi^\varepsilon, c^\varepsilon) \frac{\partial}{\partial x} f(\phi^\varepsilon, c^\varepsilon) \Big|_{x=-1}^{x=1} dt \\
&\quad - \int_0^T \int_{-1}^1 D(\phi^\varepsilon) c^\varepsilon (1 - c^\varepsilon) \left( \frac{\partial}{\partial x} f(\phi^\varepsilon, c^\varepsilon) \right)^2 dx dt,
\end{aligned}$$

and since the first term of the right side of this equation is also bounded by a constant independent of  $\varepsilon$ , we obtain the estimate

$$\int_0^T \int_{-1}^1 D(\phi^\varepsilon) c^\varepsilon (1 - c^\varepsilon) \left( \frac{\partial}{\partial x} f(\phi^\varepsilon, c^\varepsilon) \right)^2 dx dt \leq C, \tag{4.18}$$

where the constant  $C$  is independent of  $\varepsilon$ .

Multiplying both sides of (4.15) by a test function  $\zeta \in C^\infty(\overline{Q_T})$  with  $\zeta(x, T) = 0$ , and integrating the product by parts, we obtain

$$\begin{aligned} & \int_0^T \int_{-1}^1 \left[ -c^\varepsilon \zeta_t + D(\phi^\varepsilon) c^\varepsilon (1 - c^\varepsilon) \left( \frac{\partial}{\partial x} f(\phi^\varepsilon, c^\varepsilon) \right) \zeta_x \right] dx dt \\ & + \int_0^T D(\phi^\varepsilon) c^\varepsilon (1 - c^\varepsilon) \left( \frac{\partial}{\partial x} f(\phi^\varepsilon, c^\varepsilon) \right) \zeta \Big|_{x=-1}^{x=1} dt = \int_{-1}^1 c_0(x) \zeta(x, 0) dx, \end{aligned}$$

and by the estimate (4.18), we have that

$$\int_0^T \int_{-\varepsilon|\ln \varepsilon|}^{\varepsilon|\ln \varepsilon|} D(\phi^\varepsilon) c^\varepsilon (1 - c^\varepsilon) \left( \frac{\partial}{\partial x} f(\phi^\varepsilon, c^\varepsilon) \right) \zeta_x dx dt \rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0^+.$$

By taking the limit  $\varepsilon \rightarrow 0^+$ , we see that there exists a limit function  $c(x, t)$  such that, at least for a subsequence,

$$c^\varepsilon(x, t) \rightarrow c(x, t) \quad \text{in } L^\infty \text{ weak } *,$$

and in the region  $|x| \geq 2\varepsilon|\ln \varepsilon|$ , we have

$$c^\varepsilon(x, t) \rightarrow c(x, t) \quad \text{weakly in } H^1.$$

Thus, we have

$$\begin{aligned} & \int_0^T \int_{-1}^1 -c \zeta_t dx dt + \int_0^T \int_{-1}^{0^-} c_x \zeta_x dx dt + \int_0^T \int_{0^+}^1 2c_x \zeta_x dx dt \\ & = \int_{-1}^1 c_0(x) \zeta(x, 0) dx \end{aligned} \tag{4.19}$$

for any  $\zeta \in C^\infty(\overline{Q_T})$  with  $\zeta(\cdot, T) = 0$ .

Again, by a test-function argument, we see that the limit function  $c(x, t)$  satisfies

$$\begin{aligned} c_t &= c_{xx}, & -1 < x < 0, & \quad t > 0, \\ c_t &= 2c_{xx}, & 0 < x < 1, & \quad t > 0, \\ c(x, 0) &= c_0(x), & -1 < x < 1, & \\ c_x(-1, t) &= c_x(1, t) = 0, & t > 0. & \end{aligned} \tag{4.20}$$

To specify the interface condition on  $x = 0$ , we notice that (4.19) implies that

$$\begin{aligned} & \int_0^T \int_{-1}^{0^-} \left[ -(\zeta c)_t + (\zeta c_x)_x \right] dx dt + \int_0^T \int_{0^+}^1 \left[ -(\zeta c)_t + (2\zeta c_x)_x \right] dx dt \\ & = \int_{-1}^1 c_0(x) \zeta(x, 0) dx. \end{aligned} \tag{4.21}$$

Taking  $\zeta \in C^\infty(\overline{Q_T})$  with  $\zeta(x, 0) = \zeta(x, T) = \zeta(\pm 1, t) = 0$  in (4.21), we obtain

$$\int_0^T \zeta(0, t) (c_x^- - 2c_x^+) dt = 0.$$

This implies that

$$c_x^- = 2c_x^+ \tag{4.22}$$

on the interface  $x = 0$ . Another interface condition (which is the same for the dynamics as for equilibrium) follows from the estimate (4.18) and  $c(x, t) > 0$ , i.e.,

$$\ln \frac{c^-}{1 - c^-} - A = \ln \frac{c^+}{1 - c^+} + A,$$

or equivalently

$$\frac{c^-(1 - c^+)}{c^+(1 - c^-)} = e^{2A}. \tag{4.23}$$

To summarize, we have

**Theorem 4.2.** *Let  $c_0(x) \in C^1[-1, 1]$  satisfy  $0 < c_0(x) < 1$  and consistency conditions  $c_{0x}(\pm 1) = 0$  and let the function  $D(\phi^\varepsilon)$  be given by (4.4). Then problem (4.13) possesses a unique solution  $c^\varepsilon(x, t)$  for any  $\varepsilon > 0$ . Moreover, the solution  $c^\varepsilon(x, t)$  converges to a function  $c(x, t)$  as  $\varepsilon \rightarrow 0$ , and the limit function  $c(x, t)$  is the unique solution to the problem (4.20) with interface conditions (4.22) and (4.23).*

Thus, we have proved that solutions of the diffused-interface problem (4.13) converge to the solution of the sharp-interface problem (4.20), (4.22) and (4.23). Physically, this is the alloy problem in which the interface remains fixed due to thermal conditions. Our result shows once again the close relationship of the phase-field and the sharp-interface models. However, for complex geometries, the phase-field approach, (4.13), remains valid when the sharp-interface model does not apply.

*Remark 4.1.* We can take  $\phi^\varepsilon(x, t) = \tanh\{(x - vt)/\varepsilon\}$  instead of  $\phi^\varepsilon(x)$  as given by (4.3). Then the same arguments can be carried out as above. In this case the interface condition (4.22) on  $x = vt$  for the concentration equation is replaced by

$$c_x^- - 2c_x^+ = -v(c^- - c^+);$$

whereas the interface conditions on the interface  $x = vt$  for  $u$  equation remains unchanged.

(2a) We now turn to consider the case when  $D(\phi^\varepsilon)$  is given by (4.5) and we investigate the behavior of the solution  $u^\varepsilon(x, t)$  of the problem (4.6) as small parameter  $\varepsilon \rightarrow 0^+$ . Note that in this case we have

$$D(\phi^\varepsilon) \sim \varepsilon^2 + O(\varepsilon^4) \quad \text{as } x < -\varepsilon |\ln \varepsilon|.$$

Unlike the situation discussed in (1a), we have degeneracy in one phase here, so the type of equation changes in the limit case as we can see below.

As in the two previous cases, if we assume that  $u_0(x) \in L^\infty(-1, 1)$ , we can obtain the estimates:

$$\|u^\varepsilon(x, t)\|_{L^\infty(Q_T)} \leq \|u_0(x)\|_{L^\infty(-1,1)}, \tag{4.24}$$

$$\sup_{t \leq T} \int_{-1}^1 (u^\varepsilon(x, t))^2 + \int_0^T \int_{-1}^1 D(\phi^\varepsilon) |u_x^\varepsilon|^2 dx dt \leq \|u_0(x)\|_{L^2(-1,1)}^2. \tag{4.25}$$

Furthermore, if we assume that  $u_0(x) \in H^1(-1, 1)$ , then the following estimate can be derived:

$$\sup_{t \leq T} \int_{-1}^1 D(\phi^\varepsilon) |u_x^\varepsilon|^2 dx + \int_0^T \int_{-1}^1 |u_t^\varepsilon|^2 dx dt \leq \|u_{0x}(x)\|_{L^2(-1,1)}^2. \tag{4.26}$$

Noting that the solution  $u^\varepsilon(x, t)$  satisfies

$$\int_0^T \int_{-1}^1 \left[ -u^\varepsilon \zeta_t + D(\phi^\varepsilon) u_x^\varepsilon \zeta_x \right] dx dt = \int_{-1}^1 u_0(x) \zeta(x, 0) dx \tag{4.27}$$

for any  $\zeta(x, t) \in C^\infty(\overline{Q_T})$  with  $\zeta(x, T) = 0$ , we may take the limit (at least for a subsequence) as  $\varepsilon \rightarrow 0^+$  in light of estimates (4.24)–(4.26). The limit function  $u(x, t)$  satisfies

$$\int_0^T \int_{-1}^1 -u \zeta_t dx dt + \int_0^T \int_0^1 u_x \zeta_x dx dt = \int_{-1}^1 u_0(x) \zeta(x, 0) dx \tag{4.28}$$

for any  $\zeta(x, t) \in C^\infty(Q_T)$  with  $\zeta(\cdot, T) = 0$ . This implies that the function  $u(x, t)$  is a solution of

$$\begin{aligned} u_t &= 0 & \text{if } -1 < x < 0, \\ u_t &= u_{xx} & \text{if } 0 < x < 1, \\ u(x, 0) &= u_0(x) & \text{if } -1 < x < 1, \\ u_x(0^+, t) &= u_x(1, t) = 0 & \text{if } t > 0. \end{aligned} \tag{4.29}$$

It may be worth noting here that unlike case (1a), the solution  $u(x, t)$  of (4.29) may not necessarily be continuous across the interface  $x = 0$  because of the degeneracy of the original equation.

To summarize, we have

**Theorem 4.3.** *Let  $u_0(x) \in C^1[-1, 1]$  satisfy consistency conditions  $u_{0x}(\pm 1) = 0$  and let the function  $D(\phi^\varepsilon)$  be given by (4.5). Then the problem (4.6) possesses a unique solution  $u^\varepsilon(x, t)$  for any  $\varepsilon > 0$ . Moreover, the solution  $u^\varepsilon(x, t)$  converges to a function  $u(x, t)$  as  $\varepsilon \rightarrow 0$ , and the limit function  $u(x, t)$  is a solution to the problem (4.29).*

*Remark 4.2.* If we take  $\phi^\varepsilon(x, t) = \tanh\{(x - vt)/\varepsilon\}$ , then in the case  $v < 0$ , the problem (4.29) is satisfied by the limit function  $u(x, t)$  in the domains  $\{x < vt\}$  and  $\{x > vt\}$ , and  $u_x^\pm = 0$  on the interface  $x = vt$ . However, if  $v > 0$ , we have non-uniqueness in the region  $0 < x < vt, t > 0$  for the limit function  $u(x, t)$ .

(2b)  $D(\phi^\varepsilon)$  is given by (4.5) when the problem (4.13) can be treated as problem (4.6) was. For brevity we do not duplicate this argument here. Instead, we remark that the limit function  $c(x, t)$  satisfies the same equations as  $u(x, t)$  does, regardless of whether the constant  $A$  vanishes in the original equation. Again, this fact is a consequence of the degeneracy.

### 5. A Steady-State Problem with Constant Temperature

An important special case of the formal asymptotic analysis of Section 3 is that of the one-dimensional steady state at constant temperature. The rigorous verification of this problem is important for several reasons: (a) It establishes rigorously the phase diagram (which of course is defined only in the absence of dynamic and geometric considerations). (b) It establishes (at least in the steady state) the nature of the interface, namely, that it is in fact similar to a tanh function, with interface thickness  $\varepsilon$ .

The time-independent, one-dimensional simplified version of (3.1)–(3.3) subject to constant temperature and boundary conditions can be stated as

$$\begin{aligned} \varepsilon^2 \phi'' + 2\phi(1 - \phi^2) + 2\varepsilon(a + bc) &= 0 \quad \text{in } (-1, 1), \\ c' + Ac(1 - c)\phi' &= 0 \quad \text{in } (-1, 1), \\ \phi(\pm 1) &= \tanh \frac{\pm 1}{\varepsilon}, \\ c(-1) &= \sigma_-, \end{aligned} \tag{5.1}$$

where  $a, b, A$  and  $\sigma_-$  are constants with  $\sigma_0$ , and  $\varepsilon > 0$  is a small parameter.

For any positive value of  $\varepsilon$ , the system (5.1) is solvable. In fact, the second equation of (5.1) can be solved by finding  $c$  in terms of  $\phi$  as

$$c = \frac{e^{\bar{A} - A\phi}}{1 + e^{\bar{A} - A\phi}}, \tag{5.2}$$

where

$$\bar{A} = \ln \frac{\sigma_-}{1 - \sigma_-} - A\phi(-1). \tag{5.3}$$

Substituting  $c$  into the first equation of (5.1), we obtain a second-order equation for  $\phi$ , with boundary values at  $x = \pm 1$ , which is solvable.

Using  $L^\infty$  bounds, monotonicity properties and arguments employed in the Section 6, we can prove (see Figure 3 and [CX2])

**Theorem 5.1.** *Let  $0 < \sigma_- < 1$  and the pair  $(\phi^\varepsilon(x), c^\varepsilon(x))$  be a solution of the ordinary differential equation system (5.1) for any  $\varepsilon > 0$ . Then there exists a  $x(0) \in (-1, 1)$  such that, as  $\varepsilon \rightarrow 0^+$ ,*

$$\begin{aligned} \phi^\varepsilon(x) &\rightarrow -1 + 2H(x - x(0)), \\ c^\varepsilon(x) &\rightarrow \begin{cases} \sigma_- & \text{if } x < x(0), \\ \sigma_+ & \text{if } x > x(0), \end{cases} \end{aligned}$$

where the function  $H(x)$  is the Heaviside function,  $\sigma_-$  is given in (5.1) and

$$\sigma_+ = 1 - (1 - \sigma_-)e^{-2aA/b}.$$

**6. A Partial Differential Equation System with Constant Temperature**

In this section we present a rigorous treatment of the phase-alloy system (3.1)–(3.3) with  $E(c) = 1$  at constant temperature in one spatial dimension. Once again, we assume that all parameters are fixed except  $\varepsilon$ . Within this setting, we prove rigorously one special case of the formal results in Section 3. The equations have the form

$$\phi_t = \phi_{xx} + \frac{2}{\varepsilon^2} \left\{ \phi(1 - \phi^2) + \varepsilon(a + bc) \right\}, \tag{6.1}$$

$$c_t = \frac{\partial}{\partial x} \left\{ c(1 - c) \frac{\partial}{\partial x} \left[ A\phi + \ln \frac{c}{1 - c} \right] \right\} \tag{6.2}$$

in  $Q_T \equiv (-1, 1) \times (0, T)$ , subject to the boundary and initial conditions

$$\phi(x, 0) = \tanh \frac{x}{\varepsilon}, \tag{6.3}$$

$$\phi(\pm 1, t) = \tanh \frac{\pm 1}{\varepsilon}, \tag{6.4}$$

$$c(x, 0) = c_0(x), \tag{6.5}$$

$$c_x(\pm 1, t) = 0, \tag{6.6}$$

where  $a, b$  and  $A$  are constants, and the function  $c_0(x) \in C^1[0, 1]$  with  $0 < c_0(x) < 1$  and  $c_{0x}(\pm 1) = 0$  and  $\varepsilon > 0$  is a small parameter.

In this section we first state an existence and uniqueness theorem for the system (6.1)–(6.6). Then we investigate the behavior of the solution  $(\phi^\varepsilon, c^\varepsilon)$  of (6.1)–(6.6) as the parameter  $\varepsilon \rightarrow 0^+$ . The main theorem we prove is

**Theorem 6.1.** *Assume that  $c_0(x) \in C^1[-1, 1]$  with  $0 < c_0(x) < 1$  and  $c_{0x}(\pm 1) = 0$ . Let  $(c^\varepsilon, \phi^\varepsilon)$  be the solution of (6.1)–(6.6). Then there exist two functions  $S(t) \in H^1(0, T_*)$  and  $c(x, t) \in L^\infty(Q_{T_*})$  such that, as  $\varepsilon \rightarrow 0$ ,*

$$c^\varepsilon(x, t) \rightarrow c(x, t) \quad L^\infty\text{-weak}^* \quad \text{in } Q_{T_*},$$

$$\phi^\varepsilon(x, t) \rightarrow \begin{cases} -1, & \text{if } -1 < x < S(t), \\ +1, & \text{if } S(t) < x < 1, \end{cases}$$

and  $(S(t), c(x, t))$  satisfies

$$c_t = c_{xx} \quad \text{if } (x, t) \in Q_{T_*} \setminus \{(S(t), t)\},$$

satisfies the interface conditions

$$[c_x]^\pm = -[c]^\pm S'(t), \quad 0 < t \leq T_*,$$

$$\frac{2}{3} S'(t) = -2a - \frac{b}{A} \ln \frac{1 - c^+}{1 - c^-}, \quad 0 < t \leq T_*,$$

$$\left[ \ln \frac{c}{1-c} \right]_{-}^{+} = -2A, \quad 0 < t \leq T_*$$

on the interface  $x = S(t)$  and satisfies the boundary and initial conditions (6.5) and (6.6), where  $T_* > 0$  is the first time such that either  $T_* = T$ , or  $S(T_*) = -1$ , or  $S(T_*) = 1$ .

This theorem will be proved in Section 6.3 (see Theorems 6.7 and 6.8).

6.1. Existence and Uniqueness Results for  $\varepsilon > 0$

We now state the existence and uniqueness theorem for problem (6.1)–(6.6) with  $\varepsilon > 0$ . We have

**Theorem 6.2.** *There exists a unique solution  $\{\phi, c\}$  of the problem (6.1)–(6.6) for the function  $c_0(x) \in C^1[0, 1]$  with  $0 < c_0(x) < 1$  and  $c_{0x}(\pm 1) = 0$  for any  $\varepsilon > 0$ .*

This theorem can be proved by a fixed-point argument and energy-type estimates. For brevity it is not proved here.

6.2. Properties of a Solution  $(\phi^\varepsilon, c^\varepsilon)$  to (6.1)–(6.6)

To investigate the limit behavior of the solution  $(\phi^\varepsilon, c^\varepsilon)$ , we need to obtain some properties and also a priori estimates for  $(\phi^\varepsilon, c^\varepsilon)$ . First, by virtue of the maximum and comparison principles, we can derive the  $L^\infty$ -estimates

$$0 < c^\varepsilon(x, t) < 1, \tag{6.7}$$

$$-1 - 2\varepsilon(|a| + |b|) \leq \phi^\varepsilon(x, t) \leq 1 + 2\varepsilon(|a| + |b|). \tag{6.8}$$

We next prove the following energy estimate which will be used in the limit process as  $\varepsilon \rightarrow 0^+$  in Section 6.3. First, we show that  $\phi^\varepsilon(x, t)$  is approximately equal to  $\tanh\{(x - S(t))/\varepsilon\}$  for some function  $S(t) \in C^\alpha$ ,  $\alpha \in [\frac{1}{2}, 1)$ . To do this, we first restrict  $t$  to the interval  $[0, T_\varepsilon]$ , where

$$T_\varepsilon = \sup \left\{ t \in [0, T] \mid \int_0^t |\phi_x^\varepsilon(\pm 1, \tau)| d\tau \leq \varepsilon^{-\nu} \right\},$$

and  $0 < \nu < \frac{1}{2}$  is a small number (with no loss of generality, we assume that  $\int_0^{T_\varepsilon} |\phi_x^\varepsilon(\pm 1, t)| dt \geq 1$ ). In the interval  $[0, T_\varepsilon]$ , we can obtain the a priori bound for  $\int_0^{T_\varepsilon} |\phi_x^\varepsilon(\pm 1, t)| dt$ , which is independent of  $\varepsilon$ . We then conclude that  $T_\varepsilon = T$  and so obtain the energy-type estimate:

**Lemma 6.3.** *Let  $(\phi^\varepsilon, c^\varepsilon)$  be a solution of (6.1)–(6.6). Assume that  $bA < 0$ ; then*

$$\begin{aligned} & \sup_{t \leq T_\varepsilon} \int_{-1}^1 \left[ \frac{\varepsilon}{2} \phi_x^2 + \frac{1}{2\varepsilon} (1 - \phi^2)^2 \right] dx + \iint_{Q_{T_\varepsilon}} \varepsilon \phi_t^2 dx dt \\ & \quad + \frac{-2b}{A} \iint_{Q_{T_\varepsilon}} c(1-c) \left\{ \left( A\phi + \ln \frac{c}{1-c} \right)_x \right\}^2 dx dt \tag{6.9} \\ & \leq C \int_0^{T_\varepsilon} |\phi_x(\pm 1, t)| dt, \end{aligned}$$

where the constant  $C$  is independent of  $\varepsilon$ .

**Proof.** We omit the superscript and subscript  $\varepsilon$ , i.e., we write  $(\phi^\varepsilon, c^\varepsilon)$  as  $(\phi, c)$  and  $T_\varepsilon$  as  $T$  in the proof of this lemma.

By a direct calculation of the integral

$$\int_0^T \frac{d}{dt} \int_{-1}^1 \left[ \frac{\varepsilon}{2} \phi_x^2 + \frac{1}{2\varepsilon} (1 - \phi^2)^2 \right] dx dt,$$

by using integration by parts, and by using the equation for  $\phi$  and boundary and initial conditions, we find

$$\begin{aligned} & \sup_{t \leq T} \int_{-1}^1 \left[ \frac{\varepsilon}{2} \phi_x^2 + \frac{1}{2\varepsilon} (1 - \phi^2)^2 \right] dx + \iint \varepsilon \phi_t^2 dx dt \\ & \leq 2 \int_{-1}^1 [\phi(x, T) - \phi(x, 0)] dx + 2b \iint_{Q_T} c \phi_t dx dt. \end{aligned} \quad (6.10)$$

Note that we have the identities

$$\begin{aligned} \iint_{Q_T} c \phi_t dx dt &= \int_{-1}^1 c \phi \Big|_{t=0}^{t=T} dx - \frac{1}{A} \iint_{Q_T} c_t (A\phi) dx dt \\ &= \int_{-1}^1 c \phi \Big|_{t=0}^{t=T} dx - \frac{1}{A} \iint_{Q_T} c_t \left( A\phi + \ln \frac{c}{1-c} \right) dx dt \\ &\quad + \frac{1}{A} \iint_{Q_T} c_t \ln \frac{c}{1-c} dx dt \end{aligned}$$

with

$$\iint_{Q_T} c_t \ln \frac{c}{1-c} dx dt = \int_{-1}^1 [s \ln s + (1-s) \ln(1-s)] \Big|_{s=c(x,0)}^{s=c(x,T)} dx,$$

$$\begin{aligned} & \iint_{Q_T} c_t \left( A\phi + \ln \frac{c}{1-c} \right) dx dt \\ &= \iint_{Q_T} \left\{ c(1-c) \left( A\phi + \ln \frac{c}{1-c} \right)_x \right\}_x \left( A\phi + \ln \frac{c}{1-c} \right) dx dt \\ &= \int_0^T c(1-c) \left( A\phi + \ln \frac{c}{1-c} \right)_x \left( A\phi + \ln \frac{c}{1-c} \right) \Big|_{x=-1}^{x=1} dt \\ &\quad - \iint_{Q_T} c(1-c) \left\{ \left( A\phi + \ln \frac{c}{1-c} \right)_x \right\}_x^2 dx dt. \end{aligned}$$

Thus (6.10) yields

$$\begin{aligned} & \sup_{t \leq T} \int_{-1}^1 \left[ \frac{\varepsilon}{2} \phi_x^2 + \frac{1}{2\varepsilon} (1 - \phi^2)^2 \right] dx + \int \int_{Q_T} \varepsilon \phi_t^2 dx dt \\ & \quad + \frac{-2b}{A} \int \int_{Q_T} c(1 - c) \left\{ \left( A\phi + \ln \frac{c}{1 - c} \right)_x \right\}^2 dx dt \\ & \leq 2 \int_{-1}^1 [\phi(x, T) - \phi(x, 0)] dx + 2b \int_{-1}^1 c\phi \Big|_{t=0}^{t=T} dx \\ & \quad + \frac{2b}{A} \int \int_{Q_T} c_t \ln \frac{c}{1 - c} dx dt \\ & \quad + \int_0^T c(1 - c) \left( A\phi + \ln \frac{c}{1 - c} \right)_x \left( A\phi + \ln \frac{c}{1 - c} \right) \Big|_{x=-1}^{x=1} dt. \end{aligned}$$

By the estimates (6.7), (6.8), this inequality gives the desired result.  $\square$

**Lemma 6.4.** *A solution  $\phi^\varepsilon(x, t)$  of (6.1)–(6.6) has the property that*

$$\phi(x + 1 - r, t) - \phi(x, t) + O(\varepsilon) \geq 0$$

for any  $r$  with  $-1 < x < r < 1$ .

**Proof.** Let

$$\Phi(x, t) \equiv \phi(x + 1 - r, t) - \phi(x, t) + O(\varepsilon).$$

Then  $\Phi(x, t)$  satisfies the inequality

$$\Phi_t - \Phi_{xx} + \frac{2}{\varepsilon^2} [B - \hat{f}(x, t)] \Phi \geq 0,$$

and, by estimate (6.8), the boundary and initial conditions

$$\Phi(-1, t) \geq 0, \quad \Phi(r, t) \geq 0, \quad \Phi(x, 0) \geq 0$$

for  $-1 < x < r < 1$ , where

$$\hat{f}(x, t) = \int_0^1 f'(\tau\phi(x + 1 - r, t) + (1 - \tau)\phi(x, t)) d\tau,$$

$f = \phi - \phi^3$  and  $B \geq \|\hat{f}\|_{L^\infty(Q_T)} + 1$ . Hence, the comparison principle gives the desired inequality.  $\square$

**Lemma 6.5.** *A solution  $\phi^\varepsilon(x, t)$  of (6.1)–(6.6) has the property*

$$\|\varepsilon^2 \phi_x^2(\cdot, t) - (1 - \phi^2(\cdot, t))^2\|_{L^\infty(-1, 1)} \leq C\varepsilon^{\frac{1}{2} - \nu} h(t) + C\varepsilon^{1 - \nu},$$

where the constant  $C$  and the bound of  $\|h(t)\|_{L^2(0, T)}$  are independent of  $\varepsilon$ .

**Proof.** We again omit the superscript and subscript  $\varepsilon$  for brevity. The equation for  $\phi$  yields

$$\left[ \varepsilon^2 \phi_x^2 - (1 - \phi^2)^2 \right]_x = 2\varepsilon^2 \phi_x \phi_t - 4\varepsilon(a + bc)\phi_x.$$

Integrating this equality over  $(x, r) \subset (-1, 1)$ , we obtain

$$\begin{aligned} &\varepsilon^2 \phi_x^2(r, t) - (1 - \phi^2)^2(r, t) \\ &= \varepsilon^2 \phi_x^2(x, t) - (1 - \phi^2)^2(x, t) + 2\varepsilon^2 \int_x^r \phi_x \phi_t dx - 4\varepsilon \int_x^r (a + bc)\phi_x dx, \end{aligned}$$

and consequently the inequality

$$\begin{aligned} &|\varepsilon^2 \phi_x^2(r, t) - (1 - \phi^2)^2(r, t)| \\ &\leq |\varepsilon^2 \phi_x^2(x, t) - (1 - \phi^2)^2(x, t)| + 2\varepsilon^2 \left( \int_x^r \phi_x^2 dx \right)^{1/2} \left( \int_x^r \phi_t^2 dx \right)^{1/2} \\ &\quad + 4\varepsilon \left[ 2|a| + \sqrt{2}|b| \left( \int_x^r c\phi_x^2 dx \right)^{1/2} \right]. \end{aligned}$$

Integrating with respect to the  $x$  variable over  $(-1, 1)$  and using Lemma 6.3, we obtain

$$|\varepsilon^2 \phi_x^2(r, t) - (1 - \phi^2)^2(r, t)| \leq \varepsilon \int_{-1}^1 \left[ \varepsilon \phi_x^2 + \varepsilon^{-1} (1 - \phi^2)^2 \right] dx + O(\varepsilon^{\frac{1}{2}-\nu})h(t),$$

where  $h(t) \in L^2(0, T)$ ,  $\|h(t)\|_{L^2}$  is bounded and the bound is independent of  $\varepsilon$ . This proves the desired result.  $\square$

To discuss the limit as  $\varepsilon$  approaches zero and obtain interface conditions of the limit problem, we need to obtain a further estimate for  $\phi^\varepsilon(x, t)$ . To do this, we first discuss the level curves of  $\phi^\varepsilon(x, t)$ . Let  $\pm \frac{1}{2}$  be noncritical values of the function  $\phi^\varepsilon(x, t)$ . Thus Sard's lemma and the implicit function theorem imply that  $\phi^\varepsilon(x, t) = \pm \frac{1}{2}$  are composed of finitely many differentiable curves in  $Q_T$ . We denote them by  $S^\varepsilon(\pm \frac{1}{2}, t)$ . By Lemma 6.5, we see that for almost every  $t \in (0, T)$  and for a subsequence of  $\varepsilon$  (still denote by  $\varepsilon$  for brevity), we have

$$\varepsilon \phi_x^\varepsilon(x, t) \geq k > 0$$

on the region  $\{(x, t) \mid |\phi^\varepsilon| \leq \frac{1}{2}\}$  as  $\varepsilon$  is small. The continuity of  $\phi_x^\varepsilon(x, t)$  then implies that  $\phi_x^\varepsilon > 0$  and so for every  $\delta \in (-\frac{1}{2}, \frac{1}{2})$ , there exists a unique differentiable curve  $x = S^\varepsilon(\delta, t)$  such that

$$\phi^\varepsilon(S^\varepsilon(\delta, t), t) = \delta. \tag{6.11}$$

For any  $\delta(\varepsilon) \in (-\frac{1}{2}, \frac{1}{2})$ , we define

$$S^\varepsilon(t) \equiv S^\varepsilon(\delta(\varepsilon), t).$$

Integrating the ordinary differential equation suggested by Lemma 6.5, we obtain

$$\left| \phi^\varepsilon(x, t) - \tanh \frac{x - S^\varepsilon(t) + \varepsilon \mu(\varepsilon)}{\varepsilon} \right| \leq M(\varepsilon)h(t) \tag{6.12}$$

for almost every  $t \in (0, T_\varepsilon)$  and uniformly in  $x \in (-1, 1)$ , where  $\tanh(\mu(\varepsilon)) = \delta(\varepsilon)$  and  $M(\varepsilon) \rightarrow 0$  as  $\varepsilon \rightarrow 0$ .

This also implies, by the boundary condition of  $\phi^\varepsilon$ , that

$$\frac{\pm 1 - S^\varepsilon(t)}{\varepsilon} \rightarrow \pm\infty$$

as  $\varepsilon \rightarrow 0^+$  for almost every  $t \in (0, T_\varepsilon)$ .

We now stretch the  $x$  variable by

$$z \equiv \frac{x - S^\varepsilon(t)}{\varepsilon}, \quad z_\pm \equiv \frac{\pm 1 - S^\varepsilon(t)}{\varepsilon}$$

and define two functions  $\hat{\phi}^\varepsilon$  and  $\hat{c}^\varepsilon$  by

$$\hat{\phi}^\varepsilon(z, t) \equiv \phi^\varepsilon(\varepsilon z + S^\varepsilon(t), t), \tag{6.13}$$

$$\hat{c}^\varepsilon(z, t) \equiv c^\varepsilon(\varepsilon z + S^\varepsilon(t), t). \tag{6.14}$$

Our aim is to show

**Lemma 6.6.** *Let  $\phi^\varepsilon$  be a solution of (6.1)–(6.6) and  $\hat{\phi}^\varepsilon(z, t)$  be given by (6.13). Then*

$$\int_0^{T_\varepsilon} \left[ (\hat{\phi}_z^\varepsilon)^2 - (1 - (\hat{\phi}^\varepsilon)^2)^2 \right] \Big|_{z=\hat{z}_-}^{z=\hat{z}_+} \leq C\varepsilon^2 \int_0^{T_\varepsilon} |\phi_x^\varepsilon(\pm 1, t)| dt, \tag{6.15}$$

where  $\hat{z}_- \leq -|\ln \varepsilon|$ ,  $\hat{z}_+ \geq |\ln \varepsilon|$  and the constant  $C$  is independent of  $\varepsilon$ .

**Proof.** Again, we write  $\hat{\phi}^\varepsilon$  as  $\hat{\phi}$ ,  $\hat{c}^\varepsilon$  as  $c$  and  $T_\varepsilon$  as  $T$ . Let

$$\psi(z) = \psi^0(z) + \varepsilon\psi^1(z) = \left( \eta\psi_i^0 + (1 - \eta)\psi_o^0 \right) + \varepsilon \left( \eta\psi_i^1 + (1 - \eta)\psi_o^1 \right),$$

where

$$\begin{aligned} \psi_i^0(z) &= \tanh(z + \mu(\varepsilon)), \\ \psi_o^0(z) &= \begin{cases} 1, & \text{if } z > 0, \\ -1 & \text{if } z < 0; \end{cases} \end{aligned}$$

$\psi_i^1(z, t)$  is a solution of the problem

$$\begin{aligned} \psi_{izz}^1 + 2\left(1 - 3(\psi_i^0)^2\right)\psi_i^1 + 2(a + b\hat{c}) &= 0 \quad \text{in } (z_-, z_+), \\ \psi_i^1(0) &= 0, \end{aligned}$$

where

$$\psi_o^1(z, t) = \frac{1}{2}(a + b\hat{c}),$$

and where  $\eta(z) \in C^\infty(R^1)$  is a cut-off function such that

$$\eta(z) = \begin{cases} 1 & \text{if } \frac{z_-}{2} + 1 \leq z \leq \frac{z_+}{2} - 1, \\ 0 & \text{if } z \leq \frac{z_-}{2} - 1 \text{ or } z \geq \frac{z_+}{2} + 1, \end{cases}$$

and such that it is monotonically increasing from 0 to 1 if  $z < 0$  and monotonically decreasing from 1 to 0 if  $z > 0$ .

Note that the solution  $\psi_i^1(z, t)$  can be expressed by

$$\begin{aligned} \psi_i^1(z, t) = & -A(z) \int_0^z 2B(\xi) (a + b\hat{c}(\xi, t)) d\xi \\ & - B(z) \int_z^\infty 2A(\xi) (a + b\hat{c}(\xi, t)) d\xi, \end{aligned} \tag{6.16}$$

where

$$A(z) = 1 - \tanh^2(z + \mu(\varepsilon)),$$

$$B(z) = -A(z) \int_0^z \frac{1}{A^2(\xi)} d\xi.$$

Thus we obtain

$$|\psi_i^1(z, t)| \leq 2\|a + b\hat{c}\|_\infty \left( A(z) \int_0^z |B(\xi)| d\xi + |B(z)| \int_z^\infty A(\xi) d\xi \right).$$

Similary, by differentiating (6.16) with respect to  $z$ , we find that

$$|\psi_{iz}^1(z, t)| \leq 2\|a + b\hat{c}\|_\infty \left( |A'(z)| \int_0^z |B(\xi)| d\xi + |B'(z)| \int_z^\infty A(\xi) d\xi \right).$$

Therefore, we have the estimate

$$\|\psi_i^1(z, t), \psi_{iz}^1(z, t)\|_{L^\infty(Q_T)} \leq C, \tag{6.17}$$

where the constant  $C$  is independent of  $\varepsilon$ .

To justify Lemma 6.6, we need only show, by estimate (6.17), that

$$\int_0^T \left[ |\hat{\phi} - \psi^0|^2 + |\hat{\phi}_z - \psi_z^0|^2 \right] \Big|_{z=\hat{z}_-}^{z=\hat{z}_+} dt \leq C\varepsilon^2 \int_0^T |\phi_x(\pm 1, t)| dt. \tag{6.18}$$

Now consider the difference

$$\Phi(z, t) = \hat{\phi}(z, t) - \psi^0(z).$$

By noticing that

$$(\hat{\phi} - \hat{\phi}^3) - (\psi - \psi^3) = \left[ 1 - 3\psi^2 - 3\psi(\hat{\phi} - \psi) - (\hat{\phi} - \psi)^2 \right] (\hat{\phi} - \psi),$$

we see that  $\Phi(z, t)$  satisfies

$$\begin{aligned} -\Phi_{zz} + 2\left(3(\psi^0)^2 - 1\right)\Phi &= -2\left(\Phi^3 + 3\psi^0\Phi^2\right) + J(z, t) - \varepsilon^2 \frac{\partial}{\partial t} \hat{\phi}, \\ \Phi(0, t) &= 0, \\ \Phi(z_\pm, t) &= \tanh \frac{\pm 1}{\varepsilon} - (\pm 1), \end{aligned} \tag{6.19}$$

where

$$J(z, t) = 2\eta'(\psi_i^0 - \psi_o^0)_z + (\psi_i^0 - \psi_o^0) \left\{ \eta'' + 2\eta(1 - \eta) \left[ (1 + \eta)(\psi_i^0)^2 + (\eta - 2)(\psi_o^0)^2 + (1 - 2\eta)\psi_i^0\psi_o^0 \right] \right\}.$$

Multiplying the both sides of equation (6.19) by  $\phi$  and integrating the product over  $(z_-, z_+)$ , we obtain

$$\begin{aligned} & \int_{z_-}^{z_+} \left( -\Phi\Phi_{zz} + 2[3(\psi^0)^2 - 1]\Phi^2 \right) dz \\ & \leq -6 \int_{z_-}^{z_+} \psi^0\Phi^3 dz + \int_{z_-}^{z_+} J(z)\Phi dz - \varepsilon^2 \int_{z_-}^{z_+} \Phi \frac{\partial}{\partial t} \hat{\phi} dz. \end{aligned} \tag{6.20}$$

Note that we have

$$\begin{aligned} \int_{z_-}^{z_+} \left( 3(\psi^0)^2 - 1 \right) \Phi^2 dz & = \left\{ \int_{\{3(\psi^0)^2 - 1 > \delta\}} + \int_{\{3(\psi^0)^2 - 1 < \delta\}} \right\} [3(\psi^0)^2 - 1] \Phi^2 dz \\ & \geq \delta \int_{z_-}^{z_+} \Phi^2 dz + (1 + \delta) \int_{|z| \leq \sigma} \Phi^2 dz, \end{aligned}$$

where  $\sigma \leq \tanh^{-1}(1 + \delta)/3 + \mu(\varepsilon)$  and  $\delta > 0$ . Then there exist a (small) positive constant  $\delta$  and a constant  $\lambda > 0$ , such that

$$\int_{z_-}^{z_+} \Phi_z^2 dz + 2 \int_{z_-}^{z_+} \left( 3(\psi^0)^2 - 1 \right) \Phi^2 dz \geq \lambda \int_{z_-}^{z_+} \Phi_z^2 dz + 2\delta \int_{z_-}^{z_+} \Phi^2 dz,$$

and so from (6.20) we obtain the inequality

$$\begin{aligned} & \lambda \int_{z_-}^{z_+} \Phi_z^2 dz + 2\delta \int_{z_-}^{z_+} \Phi^2 dz \\ & \leq 6 \int_{z_-}^{z_+} |\psi^0\Phi|\Phi^2 dz + \frac{\delta}{4} \int_{z_-}^{z_+} \Phi^2 dz + \frac{1}{\delta} \int_{z_-}^{z_+} |J|^2 dz \\ & \quad + \varepsilon^2 \int_{z_-}^{z_+} \Phi \frac{\partial}{\partial t} \hat{\phi} dz + \Phi\Phi_z \Big|_{z_-}^{z_+}. \end{aligned}$$

Note also that

$$\|\psi^0\Phi\|_{L^\infty(z_-, z_+)} \leq 2\|\Phi\|_{L^\infty(z_-, z_+)} \leq 2\|\hat{\phi} - \psi^0\|_{L^\infty(z_-, z_+)} \leq \frac{1}{12}\delta$$

since  $\varepsilon > 0$  is suitably small. We then obtain

$$\begin{aligned} & \lambda \int_{z_-}^{z_+} \Phi_z^2 dz + \delta \int_{z_-}^{z_+} \Phi^2 dz \\ & \leq \frac{1}{\delta} \int_{z_-}^{z_+} |J|^2 dz + \frac{\varepsilon^4}{\delta} \int_{z_-}^{z_+} \left( \frac{\partial \hat{\phi}}{\partial t} \right)^2 dz + |\Phi\Phi_z| \Big|_{z_-}^{z_+}. \end{aligned} \tag{6.21}$$

The third term on the right-hand side of inequality (6.21) is exponentially small, while the integral  $\int_{z_-}^{z_+} |J|^2 dz$  can be estimated by

$$\int_{z_-}^{z_+} |J|^2 dz \leq C \left\{ \sup_{\eta \neq 0,1} [|\psi_i^0 - \psi_o^0|^2 + |\psi_{iz}^0 - \psi_{oz}^0|^2] \right\},$$

which is also exponentially small. Therefore, by integrating the inequality (6.21) over  $(0, T)$ , we obtain

$$\lambda \int_0^T \int_{z_-}^{z_+} \Phi_z^2 dz + \delta \int_0^T \int_{z_-}^{z_+} \Phi^2 dz \leq C \varepsilon^2 \int_0^T |\phi_x(\pm 1, t)| dt, \tag{6.22}$$

where we have used  $\iint_{Q_T} \varepsilon \phi_i^2 dx dt \leq C \int_0^T |\phi_x(\pm 1, t)| dt$ , which is proved in Lemma 6.3. Here the constant  $C$  is independent of  $\varepsilon$ . With estimate (6.22), we can obtain, by the same method used to obtain (6.22), the inequality

$$\int_0^T \int_{z_-}^{z_+} \Phi_{zz}^2 dz \leq C \varepsilon^2 \int_0^T |\phi_x(\pm 1, t)| dt. \tag{6.23}$$

Hence, the Sobolev imbedding theorem yields

$$\int_0^T \|\Phi(\cdot, t)\|_{L^\infty}^2 dt, \quad \int_0^T \|\Phi_z(\cdot, t)\|_{L^2}^2 dt \leq C \varepsilon^2 \int_0^T |\phi_x(\pm 1, t)| dt.$$

This proves (6.18), and so Lemma 6.6 follows.  $\square$

With the estimate  $\int_0^T |\hat{\phi}_z(z_\pm, t)|^2 dt \leq C \varepsilon^2 \int_0^T |\phi_x(\pm 1, t)| dt$ , we have

$$\begin{aligned} \int_0^{T_\varepsilon} |\phi_x(\pm 1, t)| dt &\leq (T_\varepsilon)^{1/2} \left( \int_0^{T_\varepsilon} |\phi_x(\pm 1, t)|^2 dt \right)^{1/2} \\ &\leq (T)^{1/2} \left( \int_0^{T_\varepsilon} \left| \frac{1}{\varepsilon} \hat{\phi}_z(z_\pm, t) \right|^2 dt \right)^{1/2} \leq C(T)^{1/2} \left( \int_0^{T_\varepsilon} |\phi_x(\pm 1, t)| dt \right)^{1/2}, \end{aligned}$$

and so we obtain

$$\int_0^{T_\varepsilon} |\phi_x(\pm 1, t)| dt \leq B \tag{6.24}$$

where the constant  $B$  is independent of  $\varepsilon$ . By choosing  $\varepsilon$  so small that  $B \leq \varepsilon^{-\nu}$ , we then conclude, by the definition of  $T_\varepsilon$ , that  $T_\varepsilon = T$ .

*Remark.* Once estimate (6.24) is established, we have the energy-type estimate (6.9) in Lemma 6.3, and so  $\nu = 0$  in Lemma 6.5, and the right-hand side of (6.15) is of order  $O(\varepsilon^2)$ . For any  $\delta \in (-\frac{1}{2}, \frac{1}{2})$ , differentiating the equality  $\phi^\varepsilon(S^\varepsilon(\delta, t), t) = \delta$  with respect to  $t$ , we obtain

$$\phi_x^\varepsilon(x, t) S_t^\varepsilon(\delta, t) + \phi_t^\varepsilon(x, t) = 0 \quad \text{on } x = S^\varepsilon(\delta, t),$$

and then

$$\begin{aligned} \int_0^{T_\varepsilon} \int_{-1/2}^{1/2} |S_t^\varepsilon(\delta, t)|^2 d\delta dt &= \int_0^{T_\varepsilon} \int_{-1/2}^{1/2} \left| \frac{\phi_t(\dots)}{\phi_x(\dots)} \right|^2 d\delta dt \\ &= \int_0^{T_\varepsilon} \int_{S^\varepsilon(-1/2, t)}^{S^\varepsilon(1/2, t)} \frac{|\phi_t(\dots)|^2}{|\phi_x(\dots)|} dx dt \leq \frac{\varepsilon}{k} \int_0^{T_\varepsilon} \int_{S^\varepsilon(-1/2, t)}^{S^\varepsilon(1/2, t)} |\phi_t(\dots)|^2 dx dt \leq C, \end{aligned}$$

where the constant  $C$  is independent of  $\varepsilon$ . Thus there exists a small  $\delta(\varepsilon) \in (-\frac{1}{2}, \frac{1}{2})$  such that

$$\int_0^{T_\varepsilon} |S_t^\varepsilon(\delta(\varepsilon), t)|^2 dt \leq C. \tag{6.25}$$

### 6.3. Limit Process as $\varepsilon \rightarrow 0^+$

We are now in a position to consider a limit process as  $\varepsilon \rightarrow 0^+$  and to prove our main theorem. We first show

**Theorem 6.7.** *Let  $(c^\varepsilon, \phi^\varepsilon)$  be the solution of (6.1)–(6.6). Then there exist two functions  $S(t) \in H^1(0, T_\sigma)$  and  $c(x, t) \in L^\infty(Q_{T_\sigma})$  such that, for a subsequence  $\varepsilon_j$  of  $\varepsilon$ ,*

$$\begin{aligned} c^{\varepsilon_j}(x, t) &\rightarrow c(x, t) && L^\infty\text{-weak}^* \text{ in } Q_{T_\sigma}, \\ S^{\varepsilon_j}(t) &\rightarrow S(t) && \text{uniformly in } [0, T_\sigma], \\ S^{\varepsilon_j}(t) &\rightarrow S(t) && \text{weakly in } H^1(0, T_\sigma), \end{aligned} \tag{6.26}$$

as  $\varepsilon_j \rightarrow 0$  (or  $j \rightarrow \infty$ )

$$\lim_{j \rightarrow \infty} \phi^{\varepsilon_j}(x, t) = \begin{cases} -1 & \text{if } -1 < x < S(t), \\ +1 & \text{if } S(t) < x < 1 \end{cases} \tag{6.27}$$

and  $c(x, t)$  satisfies

$$c_t = c_{xx} \quad \text{if } (x, t) \in Q_{T_\sigma} \setminus \{(S(t), t)\}, \tag{6.28}$$

where

$$T_\sigma = \sup \{ t \mid -1 - S^\varepsilon(\tau) \leq -\sigma, 1 - S^\varepsilon(\tau) \geq \sigma \quad \forall \sigma \geq 2\varepsilon |\ln \varepsilon|, \tau \leq t \}.$$

**Proof.** The convergence (6.26) can be obtained by estimates (6.7) and (6.25) established in the previous subsections, while (6.27) is a consequence of Lemma 6.6. To show (6.28), we use a test function argument. Multiplying the equation for  $c(x, t)$  by  $\zeta(x, t)$  and integrating over  $Q_{T_\sigma}$ , we obtain

$$\begin{aligned} &\int_0^{T_\sigma} \int_{-1}^1 \left\{ -c^\varepsilon \zeta_t + c^\varepsilon (1 - c^\varepsilon) \left( \frac{\partial}{\partial x} g(\phi^\varepsilon, c^\varepsilon) \right) \zeta_x \right\} dx dt \\ &+ \int_0^{T_\sigma} \zeta c^\varepsilon (1 - c^\varepsilon) \frac{\partial}{\partial x} g(\phi^\varepsilon, c^\varepsilon) \Big|_{x=-1}^{x=1} = \int_{-1}^1 c_0(x) \zeta(x, 0) dx, \end{aligned}$$

where  $\zeta \in C^\infty(Q_{T_\sigma})$  with  $\zeta(x, T_\sigma) = 0$  and

$$g(\phi, c) = A\phi + \ln \frac{c}{1-c}.$$

Note that

$$\begin{aligned} & \int_0^{T_\sigma} \int_{-1}^1 c^\varepsilon (1 - c^\varepsilon) \left( \frac{\partial}{\partial x} g(\phi^\varepsilon, c^\varepsilon) \right) \zeta_x \, dx \, dt \\ &= \int_0^{T_\sigma} \left( \int_{|x-S^\varepsilon| > \varepsilon |\ln \varepsilon|} + \int_{|x-S^\varepsilon| < \varepsilon |\ln \varepsilon|} \right) c^\varepsilon (1 - c^\varepsilon) \zeta_x \frac{\partial}{\partial x} g(\phi^\varepsilon, c^\varepsilon) \, dx \, dt \end{aligned} \tag{6.29}$$

and the second term on the right-hand side of (6.29) approaches zero as  $\varepsilon$  goes to zero by virtue of Lemma 6.3. (By the definition of  $T_\sigma$ , we see that  $|\pm 1 - S^\varepsilon(t)| > \varepsilon |\ln \varepsilon|$ .) Letting  $\varepsilon \rightarrow 0^+$ , we have

$$\begin{aligned} & \int_0^{T_\sigma} \int_{-1}^1 -c \zeta_t \, dx \, dt + \left\{ \int_0^{T_\sigma} \int_{-1}^{S(t)-} + \int_0^{T_\sigma} \int_{S(t)+}^1 \right\} c_x \zeta_x \, dx \, dt \\ &= \int_{-1}^1 c_0(x) \zeta(x, 0) \, dx, \end{aligned} \tag{6.30}$$

for  $\zeta \in C^\infty(Q_{T_\sigma})$  with  $\zeta(x, T_\sigma) = 0$ . This implies that the limit function  $c(x, t)$  satisfies

$$c_t = c_{xx} \quad \text{if } x \neq S(t). \quad \square \tag{6.31}$$

The following theorem provides the interface conditions for two limit functions  $c(x, t)$  and  $S(t)$  on  $x = S(t)$

**Theorem 6.8.** *The limit functions  $S(t)$  and  $c(x, t)$  satisfy the following interface conditions on  $x = S(t)$ :*

$$[c_x]_-^+ = -[c]_-^+ S'(t), \quad 0 < t \leq T_\sigma, \tag{6.32}$$

$$\frac{2}{3} S'(t) = -2a - \frac{b}{A} \ln \frac{1-c^+}{1-c^-}, \quad 0 < t \leq T_\sigma, \tag{6.33}$$

$$\left[ \ln \frac{c}{1-c} \right]_-^+ = -2A, \quad 0 < t \leq T_\sigma. \tag{6.34}$$

**Proof.** For our choice of  $\sigma$ , we first note that we can take  $\hat{z}_- = -|\ln \varepsilon|$  and  $\hat{z}_+ = |\ln \varepsilon|$  in Lemma 6.6. To obtain (6.32), we choose a test function  $\zeta \in C^\infty(Q_{T_\sigma})$  with  $\zeta(x, 0) = \zeta(x, T_\sigma) = \zeta(\pm 1, t) = 0$  in (6.30). From integration by parts and equation (6.31), the identity (6.32) follows. To show (6.33), we rewrite the equation for  $\phi^\varepsilon(x, t)$  in terms of the variable  $z$ , and so  $\hat{\phi}^\varepsilon(z, t)$  satisfies

$$\varepsilon \hat{\phi}_t^\varepsilon - S_t^\varepsilon \hat{\phi}_z^\varepsilon - \frac{1}{\varepsilon} \hat{\phi}_{zz}^\varepsilon - \frac{2}{\varepsilon} \left[ \hat{\phi}^\varepsilon - (\hat{\phi}^\varepsilon)^3 \right] - 2(a + b\hat{c}^\varepsilon) = 0. \tag{6.35}$$

Multiplying equation (6.35) by  $\zeta(t) \hat{\phi}_z^\varepsilon$ , we obtain

$$\begin{aligned}
 & \int_0^{T_\sigma} \int_{-|\ln \varepsilon|}^{|\ln \varepsilon|} \left[ -S_t^\varepsilon(t) (\hat{\phi}_z^\varepsilon)^2 - 2(a + b\hat{c}^\varepsilon) \hat{\phi}_z^\varepsilon \right] \zeta(t) dz dt \\
 &= \frac{1}{\varepsilon} \int_0^{T_\sigma} \int_{-|\ln \varepsilon|}^{|\ln \varepsilon|} \left[ \hat{\phi}_{zz}^\varepsilon \hat{\phi}_z^\varepsilon + 2(\hat{\phi}^\varepsilon - (\hat{\phi}^\varepsilon)^3) \hat{\phi}_z^\varepsilon \right] \zeta(t) dz dt \quad (6.36) \\
 &\quad - \varepsilon \int_0^{T_\sigma} \int_{-|\ln \varepsilon|}^{|\ln \varepsilon|} \hat{\phi}_t^\varepsilon \hat{\phi}_z^\varepsilon \zeta(t) dz dt.
 \end{aligned}$$

The second integral on the right-hand side of (6.36) can be estimated by

$$\begin{aligned}
 & \varepsilon \int_0^{T_\sigma} \int_{-|\ln \varepsilon|}^{|\ln \varepsilon|} \hat{\phi}_t^\varepsilon \hat{\phi}_z^\varepsilon \zeta(t) dz dt = \varepsilon \int_0^{T_\sigma} \int_{S^\varepsilon - \varepsilon |\ln \varepsilon|}^{S^\varepsilon + \varepsilon |\ln \varepsilon|} \phi_t^\varepsilon \phi_x^\varepsilon \zeta(t) dx dt \\
 & \leq \left( \int_0^{T_\sigma} \int_{S^\varepsilon - \varepsilon |\ln \varepsilon|}^{S^\varepsilon + \varepsilon |\ln \varepsilon|} \varepsilon (\phi_t^\varepsilon)^2 dx dt \right)^{1/2} \left( \int_0^{T_\sigma} \int_{S^\varepsilon - \varepsilon |\ln \varepsilon|}^{S^\varepsilon + \varepsilon |\ln \varepsilon|} \varepsilon (\phi_x^\varepsilon)^2 \zeta^2(t) dx dt \right)^{1/2} \\
 & \rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0^+.
 \end{aligned}$$

The first integral on the right hand side of (6.36) is of order  $O(\varepsilon)$  by Lemma 6.6.

We also have, as  $\varepsilon \rightarrow 0$ ,

$$\begin{aligned}
 & \int_0^{T_\sigma} \zeta(t) \int_{-|\ln \varepsilon|}^{|\ln \varepsilon|} S_t^\varepsilon (\hat{\phi}_z^\varepsilon)^2 dz dt \rightarrow \int_0^{T_\sigma} \zeta(t) S_t(t) dt \int_{-\infty}^{\infty} (1 - \tanh^2 z)^2 dz \\
 &= \frac{4}{3} \int_0^{T_\sigma} \zeta(t) S_t(t) dt
 \end{aligned}$$

$$2a \int_0^{T_\sigma} \zeta(t) \int_{-|\ln \varepsilon|}^{|\ln \varepsilon|} \hat{\phi}_z^\varepsilon dz dt \rightarrow 4a \int_0^{T_\sigma} \zeta(t) dt.$$

To evaluate the integral

$$\int_0^{T_\sigma} \zeta(t) \int_{-|\ln \varepsilon|}^{|\ln \varepsilon|} \hat{c}^\varepsilon \hat{\phi}_z^\varepsilon dz dt,$$

we notice that

$$\begin{aligned}
 & \int_0^{T_\sigma} \zeta(t) \int_{-|\ln \varepsilon|}^{|\ln \varepsilon|} \hat{c}^\varepsilon \left( A \hat{\phi}^\varepsilon + \ln \frac{\hat{c}^\varepsilon}{1 - \hat{c}^\varepsilon} \right)_z dz dt \\
 &= \int_0^{T_\sigma} \zeta(t) \int_{-|\ln \varepsilon|}^{|\ln \varepsilon|} \left[ A \hat{c}^\varepsilon \hat{\phi}_z^\varepsilon + \frac{\hat{c}_z^\varepsilon}{1 - \hat{c}^\varepsilon} \right] dz dt
 \end{aligned}$$

approaches zero as  $\varepsilon \rightarrow 0^+$  by Lemma 6.3, and so

$$\int_0^{T_\sigma} \zeta(t) \int_{-|\ln \varepsilon|}^{|\ln \varepsilon|} \hat{c}^\varepsilon \hat{\phi}_z^\varepsilon dz dt \rightarrow \frac{1}{A} \int_0^{T_\sigma} \zeta(t) \ln \frac{1 - c^+(S(t), t)}{1 - c^-(S(t), t)} dt$$

as  $\varepsilon \rightarrow 0^+$ .

Combining all the above estimates results in the identity (6.33).

Finally, the interface condition (6.34) follows from Lemma 6.3 and the positivity of the function  $c(x, t)$ . This completes our proof.  $\square$

To finish the proof of Theorem 6.1, we note that there exists a  $T_* > 0$  such that  $T_\sigma \rightarrow T_*$  as  $\sigma \searrow 0$ , and the limit function  $c$  satisfies the conditions (6.5) and (6.6), thereby completing the proof of Theorem 6.1.

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