An upper bound on the coarsening rate for mushy zones in a phase-field model

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Abstract

We prove an upper bound on the coarsening rate for solutions of a phase field model with arbitrarily complicated patterns of phases. The analysis is performed in a regime corresponding to the late stages of phase separation, in which the ratio between the transition layer thickness and the length scale of the pattern is small, and is also small compared to the square of the ratio between the pattern scale and the system size. The analysis extends the method of Kohn and Otto (Comm. Math. Phys. 229 (2002), 375-395) to deal with both temperature and phase fields.

1 Introduction

Phase field models are used to describe the solid-liquid phase transition of a pure material by means of two continuous field variables: the temperature u and an order parameter ϕ [2, 3, 4, 5, 6, 10, 12, 13]. The order parameter ϕ is an indicator of the local microscopic order of the material, and varies continuously from $\phi = -1$ (solid phase) to $\phi = +1$ (liquid phase). The phase field model that we consider consists of two equations written in non-dimensional form as

$$\varepsilon u_t + \frac{l}{2}\phi_t = K\Delta u, \tag{1.1}$$

$$\alpha\varepsilon\phi_t = \varepsilon\Delta\phi - \frac{1}{\varepsilon}g(\phi) + 2u. \tag{1.2}$$

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Here l, K and α are non-dimensional parameters that respectively represent latent heat, thermal diffusivity, and a relaxation time. The function $g(\phi)$ is the derivative of the double well potential $G(\phi) = \frac{1}{4}(\phi^2 - 1)^2$ which is minimized at $\phi = \pm 1$. The small parameter ε measures the thickness of the transition layers between the two phases $\{\phi \approx +1\}$ and $\{\phi \approx -1\}$ and is also related to relaxation and diffusion times and the energetic contributions of temperature fluctuations compared to phase changes. We supply more details concerning the non-dimensionalization procedure and the interpretation of parameters in an appendix.

Caginalp [3] used formal asymptotic arguments to identify sharp-interface limits of the phase field model in many limiting regimes. For the system as written above, his arguments show that as $\varepsilon \to 0$, the sharp-interface limit is the Mullins-Sekera system

$$\Delta u = 0 \qquad \text{outside } \Gamma(t) \tag{1.3}$$

$$\big[n \cdot \nabla u\big]_-^+ = -\frac{l}{K} v \qquad \text{on } \Gamma(t) \tag{1.4}$$

$$\mathit{\Delta} s\, u = -\sigma\kappa - \alpha\sigma v \qquad \text{on } \Gamma(t) \tag{1.5}$$

where $\Gamma(t) \approx \{x | \phi(x,t) = 0\}$ is the interface between the two phases, $\big[n \cdot \nabla u\big]_-^+$ is the jump of the normal derivative of u across Γ, v is the normal velocity of Γ, κ is the mean curvature of $\Gamma(t)$, $\mathit{\Delta} s$ is the difference of the entropy between the two phases, and σ is the surface tension.

This sharp-interface model keeps the same form under the scaling

$$x = \lambda \hat{x}, \quad t = \lambda^3 \hat{t}, \quad \hat{u}(\hat{x}) = \lambda u(x), \quad \hat{\alpha} = \frac{\alpha}{\lambda}. \tag{1.6}$$

In the late stages of phase change processes initiated by spinodal decomposition, or certain heterogeneously nucleated phase changes, the pattern of phases is very complicated, producing on the macroscopic level what are sometimes called "mushy zones." The structure of mushy zones is observed to coarsen in time, with average quantities such as the typical microscopic length scale of the pattern or the power spectrum exhibiting a power-law scaling behavior that is not very well understood [1]. One type of heuristic argument suggests that coarsening is somehow an asymptotically statistically self-similar process not depending on the fine details of the pattern. Then the scaling (1.6) suggests that as the length scale becomes large, the influence of α can be neglected, and the coarsening rate of the sharp-interface model should be

$$\hat{L}(t) \sim t^{1/3},$$

where $\hat{L}(t)$ is a characteristic length scale of the pattern or distribution of phases. Consequently, we expect the solution of the phase field system to have the same coarsening rate, at least when ε is sufficiently small.

One cannot expect all solutions to coarsen, due to the likely presence of fine-scale unstable equilibria for example, and anyway, in the infinite-time limit the system should typically reach a stable equilibrium and stop coarsening. But Kohn and Otto [7] have recently introduced a powerful method to obtain rigorous, universally valid *upper bounds* on intermediate-time coarsening rates that have the right power-law nature (see also [8, 9]). One of the cases treated in [7] is the Cahn-Hilliard equation, whose sharp-interface limit is the same Mullins-Sekerka system in (1.3)–(1.5) with $\alpha = 0$, see [11] for details. It is our aim in this paper to extend the method of [7] to treat the phase-field system (1.1)–(1.2), and obtain time-averaged upper bounds on the coarsening rate under physically reasonable assumptions.

We will consider the coarsening dynamics in a large cubic cell $Q := [0, a]^n \subset \mathbf{R}^n$ and with periodic boundary conditions to avoid boundary effects. As in [7], we will always consider volume-averaged integrals denoted by

$$\fint f := \frac{1}{\mathrm{vol}(Q)} \int_Q f,$$

as our goal is to obtain universal bounds independent of the size of Q. Our bounds will be valid when the transition layer thickness ε is small compared to a characteristic length scale $\hat{L}$ and the ratio $\varepsilon/\hat{L} \ll (\hat{L}/a)^2$, and therefore we are able to consider very complicated patterns of phases when $\hat{L}(t) \ll a$.

As long as the initial values are continuous and $\varepsilon < \alpha K$, the initial-value problem for the phase field system (1.1)-(1.2) is globally well posed and the solution is classical, see [2]. By (1.1) and the periodic boundary condition,

$$\frac{d}{dt}\fint (\varepsilon u + \frac{l}{2}\phi) = \fint (\varepsilon u_t + \frac{l}{2}\phi_t) = \fint K\Delta u = 0.$$

So $\fint(\varepsilon u + \frac{l}{2}\phi)$ is conserved, and we will focus on the case $\fint(\varepsilon u + \frac{l}{2}\phi) = 0$, i.e.,

$$\varepsilon \bar{u} + \frac{l}{2}\bar{\phi} = 0, \tag{1.7}$$

where $\bar{u} = \fint u$ and $\bar{\phi} = \fint \phi$. Hence we only consider those initial data that satisfy (1.7). The phase field system (1.1)–(1.2) dissipates a volume-averaged negative entropy $S(t)$ (cf. [13]), which is defined by

$$S(t) := \fint \frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon}G(\phi) + \frac{2\varepsilon}{l}u^2. \tag{1.8}$$

The time derivative of S is

$$\begin{aligned}\dot{S} &= \fint \big(-\varepsilon\Delta\phi + \frac{1}{\varepsilon}g(\phi)\big)\phi_t + \frac{4\varepsilon}{l}uu_t \\ &= \fint (2u - \alpha\varepsilon\phi_t)\phi_t + \frac{4}{l}(K\Delta u - \frac{l}{2}\phi_t)u \\ &= \fint -\frac{4K}{l}|\nabla u|^2 - \alpha\varepsilon\phi_t^2.\end{aligned}$$

So $\dot{S} \leqslant 0$ and $S(t)$ is a decreasing function of t. Note that in the sharp-interface limit, $S(t)$ corresponds to the volume-averaged *area* of the interface between the phases, and so scales as inverse to length, cf. [3, 6].

The method of Kohn and Otto involves three key steps. The first is to find a *dissipation relation* that bounds the growth rate of a suitable measure of length scale in terms of the dissipation of a dual quantity, which is negative entropy in this case. Here, as a measure of length scale we will employ the H^{-1} Sobolev norm of the scaled energy density $\varepsilon u + \frac{l}{2}\phi$. We define

$$L(t) := \left(\fint |\nabla v|^2\right)^{1/2}, \tag{1.9}$$

where v is a periodic function that satisfies

$$\Delta v = \varepsilon u + \frac{l}{2}\phi. \tag{1.10}$$

By (1.7), v exists and is uniquely determined up to a spatial constant, so L is well defined. Taking the time derivative of $L^2(t) = \fint |\nabla v|^2$, we get

$$\begin{aligned}L\dot{L} &= \fint \nabla v \nabla v_t \;=\; \fint (-\Delta v_t)v \;=\; \fint \left(-\varepsilon u_t - \frac{l}{2}\phi_t\right)v \\ &= \fint -K\Delta u\, v \;=\; \fint K\nabla u \nabla v \leqslant K\left(\fint |\nabla v|^2\right)^{1/2}\left(\fint |\nabla u|^2\right)^{1/2}.\end{aligned}$$

So

$$|\dot{L}| \leqslant K\left(\fint |\nabla u|^2\right)^{1/2} \leqslant K\left(\frac{l}{4K}(-\dot{S})\right)^{1/2},$$

that is,

$$|\dot{L}|^2 \leqslant \frac{Kl}{4}(-\dot{S}) \tag{1.11}$$

This will prove to be the required dissipation relation.

The second key step involves proving an *interpolation inequality*, of the form

$$L(t)S(t) \geqslant C_1, \tag{1.12}$$

valid under certain conditions for all $t \geq 0$. The constant $C_1 > 0$ depends only on K, l, the dimension of space n, and the form of the double-well potential, and doesn't depend on the domain Q, the parameter ε or the size of S and L. We shall find that (1.12) is valid under the conditions

$$\frac{\varepsilon}{\hat{L}} \ll 1, \qquad \frac{\varepsilon}{\hat{L}} \ll \left(\frac{\hat{L}}{a}\right)^2, \tag{1.13}$$

where $\hat{L}^{-1}$ is an upper bound for $S(0)$ and may be regarded as a length scale.

The third step in the Kohn-Otto method is an elementary ODE argument (Lemma 3 in [7]). The dissipation relation (1.11) and the interpolation inequality (1.12) together with the ODE lemma in [7] lead directly to our main result.

Theorem 1.1 *Provided that the conditions (1.13) hold, there exist positive constants C_2 and C_3 such that for any solutions $u(t,x)$ and $\phi(t,x)$ of the equations (1.1) and (1.2), if the initial data satisfy (1.7) and $\hat{L}S(0) \leqslant 1$, then*

$$⨍_0^T S(t)^2 dt \geqslant C_2 ⨍_0^T (t^{-1/3})^2 dt \quad \textit{for } T \geqslant C_3 L(0)^3. \tag{1.14}$$

The constants C_2 and C_3 depend only on K, l, n and the form of the double-well potential G, and not on ε, α, $L(0)$, or $S(0)$.

The estimate (1.14) is a time-averaged version of the (unproven) pointwise estimate $S(t) \geqslant Ct^{-1/3}$, which corresponds to an upper bound on the length scale $1/S(t)$ with the expected power-law behavior. Theorem 3.1, adapted from [7], provides time-averaged estimates on some other integral combinations of $S(t)$ and $L(t)$. By tracking the constants in the arguments of [7], we find $C_2 = \frac{1}{6}(3m)^{1/3}$ and $C_3 = 8/(3m)$ where $m = \min\{\frac{1}{4}C_1^2, C_1^4/(Kl)^2\}$.

At this point, it only remains to prove the interpolation inequality (1.12).

2 The interpolation inequality

In this section, we will prove the interpolation inequality (1.12) under the assumptions indicated above. Define periodic functions w and ψ such that

$$\Delta w = u - \bar{u} \qquad \text{and} \qquad \Delta\psi = \phi - \bar{\phi}. \tag{2.1}$$

w and ψ are determined up to a spatial constant, which we fix by requiring $\bar{w} = 0$, $\bar{\psi} = 0$. By (1.8) we have

$$⨍ \frac{2\varepsilon}{l} u^2 \leqslant S, \tag{2.2}$$

so we get

$$\Big(⨍ |u - \bar{u}|^2 \Big)^{1/2} \leqslant \Big(⨍ u^2 \Big)^{1/2} \leqslant \sqrt{\frac{l}{2\varepsilon}} \sqrt{S}, \tag{2.3}$$

The periodicity of w guarantees that $\int \nabla w = 0$. By Poincaré's inequality, together with an integration by parts justified by the periodicity of w,

$$\begin{aligned} \Big(⨍ |\nabla w|^2 \Big)^{1/2} &\leqslant Ca \Big(⨍ \sum_{i,j} \Big| \frac{\partial^2 w}{\partial x_i \partial x_j} \Big|^2 \Big)^{1/2} = Ca \Big(⨍ |\Delta w|^2 \Big)^{1/2} \\ &= Ca \Big(⨍ |u - \bar{u}|^2 \Big)^{1/2} \leqslant Ca \sqrt{\frac{l}{2\varepsilon}} \sqrt{S}, \end{aligned} \tag{2.4}$$

where C is a positive constant which depends only on the dimension of space.

By (2.1) and (1.7),

$$\Delta(\varepsilon w + \frac{l}{2}\psi) = \varepsilon(u - \bar{u}) + \frac{l}{2}(\phi - \bar{\phi}) = \varepsilon u + \frac{l}{2}\phi. \tag{2.5}$$

Comparing (2.5) with (1.10), we get

$$\begin{aligned} L(t) &= \Big(⨍ |\varepsilon \nabla w + \frac{l}{2} \nabla \psi|^2 \Big)^{1/2} \\ &\geqslant \frac{l}{2} \Big(⨍ |\nabla \psi|^2 \Big)^{1/2} - \varepsilon \Big(⨍ |\nabla w|^2 \Big)^{1/2} \\ &\geqslant \frac{l}{2} \Big(⨍ |\nabla \psi|^2 \Big)^{1/2} - Ca \sqrt{\frac{l\varepsilon}{2}} S^{1/2}, \end{aligned}$$

so

$$L(t)S(t) \geqslant \frac{l}{2} \Big(⨍ |\nabla \psi|^2 \Big)^{1/2} \Big(⨍ \frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} G(\phi) \Big) - Ca \sqrt{\frac{l\varepsilon}{2}} S^{3/2}.$$

Let us now define

$$L_1(t) = \Big(⨍ |\nabla \psi|^2 \Big)^{1/2}, \tag{2.6}$$

$$S_1(t) = ⨍ \frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} G(\phi). \tag{2.7}$$

Then

$$L(t)S(t) \geqslant \frac{l}{2}L_1S_1 - Ca\sqrt{\frac{l\varepsilon}{2}}\,S^{3/2}. \tag{2.8}$$

Now it is time to prove the interpolation inequality relating $L(t)$ and $S(t)$.

Lemma 2.1 *Given any constant $M > 0$, provided $\varepsilon_0 M$ and $\varepsilon_0 a^2 M^3$ are sufficiently small, there exists a positive constant C_1 such that whenever $0 < \varepsilon < \varepsilon_0$ and $S(0) < M$, we have*

$$L(t)S(t) \geqslant C_1 \quad \text{for all } t \geqslant 0. \tag{2.9}$$

Proof. The proof is similar to that of Lemma 1 in [7]. But our length scales L_1 and L are different from that in [7] and need a somewhat different treatment. For the sake of completeness and since we want to track every constant, especially the parameter ε, we reproduce every detail here.

Since $1 = (1-\phi^2) + \phi^2$, and

$$⨍(1-\phi^2) \leqslant \left(⨍(1-\phi^2)^2\right)^{1/2} \leqslant (4\varepsilon S_1)^{1/2}, \tag{2.10}$$

the remaining work is to estimate $⨍\phi^2$ in terms of L_1, S_1 and S.

Next, we will use the Modica-Mortola inequality. Define

$$W(\phi) = \int_0^\phi |1-t^2|\,dt. \tag{2.11}$$

We have

$$\frac{\partial W}{\partial \phi} = |1-\phi^2| = 2\sqrt{G(\phi)},$$

so

$$⨍|\nabla(W(\phi))| = ⨍|\nabla\phi|\frac{\partial W}{\partial\phi} \leqslant ⨍\frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{1}{2\varepsilon}|\frac{\partial W}{\partial\phi}|^2 \leqslant 2S_1. \tag{2.12}$$

We will use a smooth mollifier ρ which is radially symmetric, non-negative and supported in the unit ball with $\int_{\mathbf{R}^n}\rho = 1$. Let the subscript δ denote the convolution with the kernel

$$\frac{1}{\delta^n}\rho\left(\frac{\cdot}{\delta}\right).$$

The parameter δ will be optimized later. We split $⨍\phi^2$ into two parts:

$$⨍\phi^2 \leqslant 2⨍(\phi-\phi_\delta)^2 + 2⨍\phi_\delta^2. \tag{2.13}$$

Noting that

$$|\phi_1 - \phi_2|^2 \leqslant 8|W(\phi_1) - W(\phi_2)|$$

for all ϕ_1 and ϕ_2, we get the following estimate for the first term of (2.13),

$$\begin{aligned} 2\fint (\phi - \phi_\delta)^2 &\leqslant 2 \sup_{|h|\leqslant\delta} \fint (\phi(x) - \phi(x+h))^2 dx \\ &\leqslant 16 \sup_{|h|\leqslant\delta} \fint |W(\phi(x)) - W(\phi(x+h))|\, dx \\ &\leqslant 16\delta \fint |\nabla(W(\phi))| \leqslant 32\delta S_1. \end{aligned} \tag{2.14}$$

For the second term of (2.13), we need to deal with large and small values of $|\phi_\delta|$:

$$\fint \phi_\delta^2 = \fint (\phi_\delta^2 - \min\{\phi_\delta^2, 4\}) + \fint \min\{\phi_\delta^2, 4\}. \tag{2.15}$$

Since $F(\phi) := \phi^2 - \min\{\phi^2, 4\}$ is convex in ϕ, by Jensen's inequality and the fact that $\int \rho(y)dy = 1$,

$$F(\phi_\delta(x)) = F\left(\int \rho(y)\phi(x - \delta y)dy\right) \leqslant \int \rho(y) F(\phi(x - \delta y))dy.$$

So the first term of (2.15) is

$$\begin{aligned} \fint (\phi_\delta^2 - \min\{\phi_\delta^2, 4\}) &\leqslant \fint \int \rho(y) F(\phi(x - \delta y))\, dy\, dx \\ &= \int \rho(y) \fint \Big[\phi^2(x - \delta y) - \min\{\phi^2(x - \delta y), 4\}\Big]\, dx\, dy \\ &= \fint (\phi^2(x) - \min\{\phi^2(x), 4\})\, dx \\ &\leqslant \fint \frac{1}{2}(1 - \phi^2)^2 \leqslant 2\varepsilon S_1. \end{aligned} \tag{2.16}$$

For the second term of (2.15), we have

$$\fint \min\{\phi_\delta^2, 4\} \leqslant 2\fint |\phi_\delta|. \tag{2.17}$$

We know that

$$\fint |\phi_\delta| = \sup\left\{\fint \phi_\delta(x)\zeta(x)\, dx : \zeta \text{ is } Q\text{-periodic and } |\zeta(x)| \leqslant 1 \text{ a.e.}\right\}.$$

For any ζ that is Q-periodic and $|\zeta(x)| \leqslant 1$ a.e.,

$$\zeta_\delta(x) = \int \frac{1}{\delta^n}\rho\left(\frac{x-y}{\delta}\right)\zeta(y)dy.$$

So

$$\nabla\zeta_\delta(x) = \frac{1}{\delta}\int \frac{1}{\delta^n}\nabla\rho\left(\frac{x-y}{\delta}\right)\zeta(y)dy = \frac{1}{\delta}\int \nabla\rho(y)\zeta(x-\delta y)dy,$$

and hence

$$\sup|\nabla\zeta_\delta| \leqslant \beta\frac{1}{\delta}\sup|\zeta| \leqslant \beta\frac{1}{\delta},$$

where $\beta = \int |\nabla\rho|$.

$$\begin{aligned}
⨍ \phi_\delta(x)\zeta(x)\,dx &= ⨍ \phi(x)\zeta_\delta(x) \\
&= ⨍ \big(\Delta\psi - \frac{2\varepsilon}{l}\bar{u}\big)\zeta_\delta(x) \quad \text{(by (2.1) and (1.7))} \\
&= -⨍ \nabla\psi\nabla\zeta_\delta(x)\,dx - \frac{2\varepsilon}{l}\bar{u}⨍ \zeta_\delta \\
&\leqslant \left(⨍ |\nabla\psi|^2\right)^{1/2}\left(⨍ |\nabla\zeta_\delta|^2\right)^{1/2} + \frac{2\varepsilon}{l}|\bar{u}|⨍ |\zeta_\delta| \\
&\leqslant \frac{\beta}{\delta}L_1 + \sqrt{\frac{2\varepsilon S}{l}}. \qquad (2.18)
\end{aligned}$$

Taking supremum over all such ζ, we get

$$⨍ |\phi_\delta| \leqslant \frac{\beta}{\delta}L_1 + \sqrt{\frac{2\varepsilon S}{l}}. \qquad (2.19)$$

Combining these estimates, we get

$$⨍ \phi^2 \leqslant 32\delta S_1 + 4\varepsilon S_1 + 4\frac{\beta}{\delta}L_1 + 4\sqrt{\frac{2\varepsilon S}{l}}. \qquad (2.20)$$

Since δ is arbitrary, we minimize the right hand side over all $\delta > 0$ and get

$$⨍ \phi^2 \leqslant 16\sqrt{2\beta}\sqrt{L_1 S_1} + 4\varepsilon S_1 + 4\sqrt{\frac{2\varepsilon S}{l}}. \qquad (2.21)$$

Combining this estimate with (2.10), we obtain

$$1 \leqslant 16\sqrt{2\beta}\sqrt{L_1 S_1} + 4\varepsilon S_1 + 4\sqrt{\frac{2\varepsilon S}{l}} + \sqrt{4\varepsilon S_1}. \qquad (2.22)$$

Now, since S is a decreasing function of t and $S_1(t) \leqslant S(t)$ for all $t > 0$, we have

$$S_1(t) \leqslant S(t) \leqslant M \quad (t > 0).$$

Provided $\varepsilon_1 M$ is sufficiently small (depending only on l), we have

$$4\varepsilon S_1 + 4\sqrt{\frac{2\varepsilon S}{l}} + \sqrt{4\varepsilon S_1} < \frac{1}{2} \qquad (0 < \varepsilon \leqslant \varepsilon_1),$$

so

$$16\sqrt{2\beta}\sqrt{L_1 S_1} \geqslant \frac{1}{2},$$

and hence

$$L_1 S_1 \geqslant \hat{C}_1, \tag{2.23}$$

where $\hat{C}_1 = 1/(2048\beta)$. On the other hand, provided $\varepsilon_2 M \cdot (aM)^2$ is sufficiently small, (depending only on l and n), we have

$$Ca\sqrt{\frac{l\varepsilon}{2}} S^{3/2} \leqslant \frac{l}{4}\hat{C}_1 \quad (0 < \varepsilon \leqslant \varepsilon_2,\ t > 0). \tag{2.24}$$

Let $\varepsilon_0 = \min\{\varepsilon_1, \varepsilon_2\}$ and $C_1 = \frac{l}{4}\hat{C}_1$. By (2.8),

$$L(t)S(t) \geqslant \frac{l}{2} L_1(t)S_1(t) - Ca\sqrt{\frac{l\varepsilon}{2}} S^{3/2} \geqslant C_1 \quad (0 < \varepsilon \leqslant \varepsilon_0,\ t > 0). \tag{2.25}$$

3 Upper bounds

Applying the ODE argument of [7] without change, we get the main result.

Theorem 3.1 *Under the assumptions of Lemma 2.1, for any* $0 \leqslant \theta \leqslant 1$ *and* $0 < r < 3$ *satisfying* $\theta r > 1$ *and* $(1-\theta)r < 2$*, there exists positive constants* C_2 *and* C_3*, depending only on* K, l, θ, r *and the dimension of space, such that for all* $0 < \varepsilon \leqslant \varepsilon_0$

$$\fint_0^T S^{\theta r} L^{-(1-\theta)r} dt \geqslant C_2 \fint_0^T (t^{-1/3})^r dt, \ \text{if } T \geqslant C_3 L(0)^3. \tag{3.1}$$

Proof. The inequalities (1.11) and (2.9) give us

$$(\dot{L})^2 \leqslant \frac{Kl}{4}(-\dot{S}) \quad \text{and} \quad LS \geqslant C_1, \quad (0 < \varepsilon \leqslant \varepsilon_0,\ t > 0).$$

The theorem is then an immediate consequence of Lemma 3 in [7]. In particular, we obtain (1.14) by choosing $\theta = 1, r = 2$.

Appendix

To help clarify what physical conditions yield the system (1.1)–(1.2), we briefly discuss the non-dimensionalization procedure here. We begin from a dimensional version of the standard phase field system, derived following [12]. We start with a bulk free energy density f at the phase transition temperature T_0 given by

$$f(T_0, \phi) = \beta_0 G(\phi) = \frac{\beta_0}{4}(\phi^2 - 1)^2, \tag{A.1}$$

and bulk energy density given in terms of temperature T and order parameter ϕ by

$$e(T, \phi) = c_0 T + b_0 \phi. \tag{A.2}$$

Here c_0 is heat capacity and $2b_0$ is latent heat. The thermodynamic relation $\partial(f/T)/\partial(1/T) = e$ yields

$$f(T, \phi) = c_0 T \log \frac{T_0}{T} + b_0 \phi \left(1 - \frac{T}{T_0}\right) + \beta_0 \frac{T}{T_0} G(\phi). \tag{A.3}$$

The phase field system obtained from the kinetic derivation of [13], after linearizing the contribution of temperature to the phase-field evolution equation, is

$$c_0 T_t + b_0 \phi_t = K_0 \Delta T, \tag{A.4}$$

$$\alpha_0 \phi_t = \kappa_0 \Delta \phi - \frac{\beta_0}{T_0} G'(\phi) + \frac{b_0}{T_0^2}(T - T_0). \tag{A.5}$$

Here K_0 is the heat conductivity, and α_0 and κ_0 can be determined from the quantities

$$x_1 = \left(\frac{\kappa_0 T_0}{\beta_0}\right)^{1/2}, \qquad t_r = \frac{\alpha_0 T_0}{\beta_0}, \tag{A.6}$$

which respectively represent a domain wall thickness and a relaxation time for the phase field. For the system in this form, a Lyapunov function is the quantity

$$S_0 = \int_Q \frac{1}{2} \kappa_0 |\nabla \phi|^2 + \frac{\beta_0}{T_0} G(\phi) + \frac{c_0}{2T_0^2}(T - T_0)^2, \tag{A.7}$$

which has dimensions of entropy, but is not identical to the (negative) entropy involved in the kinetic derivation of [13] due to the linearization step mentioned.

We non-dimensionalize according to

$$T - T_0 = u_0 \hat{u}, \qquad x = x_0 \hat{x}, \qquad t = t_0 \hat{t}, \tag{A.8}$$

where u_0, x_0, t_0 represent typical temperature fluctuation, length and time scales, respectively. One then obtains the system (1.1)–(1.2) under the conditions that

$$\varepsilon = \frac{x_1}{x_0} = \sqrt{\frac{t_r}{\alpha t_0}} = \frac{b_0 u_0}{2\beta_0 T_0} = \frac{l}{2}\frac{c_0 u_0}{b_0} = K\frac{c_0 x_0^2}{K_0 t_0}. \tag{A.9}$$

These relations make clear the conditions under which the parameter ε is small while l, K, and α remain order one quantities: the domain wall thickness and phase relaxation time should be small compared to typical length and time scales; energetic contributions of temperature fluctuations should be small compared to those of phase changes; and the time scale t_0 should be long compared to the heat diffusion time $t_D = x_0^2 c_0/K_0$.

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