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Abstract. A Ginzburg–Landau type functional for a multi–phase system involving a diffuse interface description of the phase boundaries is presented with the following calibration property: Prescribed surface energies (possibly anisotropic) of the phase transitions are correctly recovered in the sense of a Γ–limit as the thickness of the diffuse interfaces converges to zero. Possible applications are grain boundary motion and solidification of alloys on which numerical simulations are presented.

1. Introduction

Consider a domain $\Omega \subset \mathbb{R}^d$, $d \in \{1,2,3\}$, which is subdivided into several (not necessarily connected) regions Ω_α, $\alpha \in \{1,\dots,\mathcal{M}\}$, $\mathcal{M} \in \mathbb{N}$, separated by hypersurfaces $\Gamma_{\alpha\beta}$, $1 \le \alpha < \beta \le \mathcal{M}$. The interfaces are supposed to carry energy obtained by integrating surface densities which may depend on the orientation of the hypersurface. The total energy of the system has the form

$$\mathcal{F}_{SI} = \sum_{\alpha<\beta} \int_{\Gamma_{\alpha\beta}} \sigma_{\alpha\beta}(\nu_{\alpha\beta}) d\mathcal{H}^{d-1}. \tag{1.1}$$

To avoid wetting effects is is assumed that $\sigma_{\alpha\beta} + \sigma_{\beta\delta} > \sigma_{\alpha\delta} > 0$ for each triple of phases α, β, δ.

Energies as in (1.1) can be approximated by Ginzburg–Landau energies of the form

$$\mathcal{F}_{PF} = \int_\Omega \Big(\varepsilon a(\phi, \nabla\phi) + \frac{1}{\varepsilon} w(\phi) \Big) d\mathcal{L}^d. \tag{1.2}$$

Here, $\phi = (\phi_1, \dots, \phi_\mathcal{M}) : \Omega \to \Sigma^\mathcal{M}$ with

$$\Sigma^\mathcal{M} := \Big\{ v \in \mathbb{R}^\mathcal{M} : \sum_{\alpha=1}^{\mathcal{M}} v_\alpha = 1 \text{ and } 0 \le v_\alpha \le 1 \text{ for all } \alpha = 1,\dots,\mathcal{M} \Big\}$$

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is a set of phase field variables. For each α, ϕ_α is assigned to one of the phases (labelled α and occupying Ω_α) and describes its presence in a point of Ω. The function $a(\phi, \nabla\phi)$ is a non–negative gradient term, and $w(\phi)$ is a multi–well potential with $\mathcal{M}$ minima corresponding to the phases. It is well known that such Ginzburg–Landau energies cause transition regions where the phase fields vary from one of the minima of w, i.e. from one of the phases, to another one. The thickness of the interfacial layers is of the order ε, a small length scale.

Bellettini et al. [2] showed that the Γ–limit of (1.2) as $\varepsilon \to 0$ has the form (1.1), and they proved a relation between the $\sigma_{\alpha\beta}$ and the functions a and w. Using matched asymptotic expansions, Sternberg [10] for the isotropic case and Garcke et al. [5] for the general case found the slightly simpler relation

$$\sigma_{\alpha\beta}(\nu) = \inf_p \Big\{ \int_{-1}^{1} \sqrt{w(p)a(p, p' \otimes \nu)}\, dy, \quad p \in C^{0,1}([-1,1]; \Sigma^{\mathcal{M}}),\ p(-1) = e_\alpha,\ p(1) = e_\beta \Big\} \tag{1.3}$$

where e_α and e_β are the corners of the simplex $\Sigma^{\mathcal{M}}$ corresponding to the phases α and β, i.e., $e_\eta = (\delta_{\eta\theta})_{\theta=1}^{\mathcal{M}}$ with the Kronecker symbols $\delta_{\eta\theta}$. Using numerical simulations they showed that this formula holds true for a large class of anisotropies. Vice versa, it is a non–trivial task to construct functions a and w such that the surface energies obtained via (1.3) coincide with given surface energies (which, in applications, may be known from experiments).

A possible solution has been found by the author in collaboration with H. Garcke and R. Haas (see [7]) and will be presented in the following sections. First some facts on the minimization problem (1.3), afterwards the precise aims are stated. Some additional conditions on a and w are imposed:

Definition 1.1. Let

$$T\Sigma^{\mathcal{M}} := \Big\{ v = (v_1, \dots, v_{\mathcal{M}}) \in \mathbb{R}^{\mathcal{M}} : \sum_{\alpha=1}^{\mathcal{M}} d_\alpha = 0 \Big\}.$$

The function $a : \Sigma^{\mathcal{M}} \times (T\Sigma^{\mathcal{M}})^d \to \mathbb{R}$ is an admissible gradient term if

$$a(\phi, X) \geq 0, \quad a(\phi, \eta X) = \eta^2 a(\phi, X) \quad \forall \phi \in \Sigma^{\mathcal{M}}, X \in (T\Sigma^{\mathcal{M}})^d, \eta \in \mathbb{R}, \tag{1.4}$$

$$a_{\alpha\beta}(\nu) := a(se_\beta + (1-s)e_\alpha, (e_\beta - e_\alpha) \otimes \nu) \text{ does not depend on } s \in [0,1] \quad \forall \alpha, \beta \in \{1, \dots, \mathcal{M}\}. \tag{1.5}$$

The function $w : \Sigma^{\mathcal{M}} \to \mathbb{R}$ is an admissible multi–well potential if

$$w(\phi) \geq 0\ \forall \phi \in \Sigma^{\mathcal{M}}, \quad w(\phi) = 0 \Leftrightarrow \phi \in \{e_1, \dots, e_N\}, \tag{1.6}$$

$$w(se_\beta + (1-s)e_\alpha) = w_{\alpha\beta} s^2 (1-s)^2, \quad \forall s \in [0,1],\ \alpha, \beta \in \{1, \dots, \mathcal{M}\}. \tag{1.7}$$

A minimizer of the problem in (1.3) fulfills after appropriate rescaling to some function $\phi : \mathbb{R} \to \Sigma^{\mathcal{M}}$ (cp. [5] for this procedure)

$$
\begin{aligned}
& w_{,\phi}(\phi) + a_{,\phi}(\phi, \partial_z\phi \otimes \nu) - \frac{d}{dz}\Big(a_{,X}(\phi, \partial_z\phi \otimes \nu)\nu\Big) = \boldsymbol{\lambda}, \\
& \lim_{z\to\infty} \phi(z) = e_\beta, \quad \lim_{z\to-\infty} \phi(z) = e_\alpha,
\end{aligned} \tag{1.8}
$$

where $\lambda = \frac{1}{\mathcal{M}} \sum_{i=1}^{\mathcal{M}} w_{,\phi_i}(\phi) + a_{,\phi_i}(\phi, \partial_z\phi \otimes \nu) - \frac{d}{dz}\big(a_{,X_i}(\phi, \partial_z\phi \otimes \nu)\nu\big)$ is a Lagrange multiplier and $\boldsymbol{\lambda} = \lambda(1, \dots, 1) \in \mathbb{R}^{\mathcal{M}}$. In particular, the minimization problem in (1.3) reads now

$$
\begin{aligned}
\sigma_{\alpha\beta}(\nu) = \inf_{\phi} \Big\{ \int_{\mathbb{R}} \Big(a(\phi, \partial_z\phi \otimes \nu) + w(\phi)\Big) dz, \\
\phi \in C^{0,1}(\mathbb{R}; \Sigma^{\mathcal{M}}),\ \lim_{z\to-\infty} \phi(z) = e_\alpha,\ \lim_{z\to\infty} \phi(z) = e_\beta \Big\}.
\end{aligned} \tag{1.9}
$$

Lemma 1.2. Consider a function of the form

$$
\phi(z) = \chi(z)e_\beta + (1 - \chi(z))e_\alpha. \tag{1.10}
$$

Then ϕ solves (1.8) for admissible functions a and w if

$$
\chi(z) = \frac{1}{2}\Big(1 + \tanh\big(\sqrt{\tfrac{w_{\alpha\beta}}{a_{\alpha\beta}(\nu)}}\,\frac{z}{2}\big)\Big) \quad \text{and if} \tag{1.11}
$$

$$
\lambda = w_{,\phi_i} + |\chi'|^2 a_{,\phi_i} - \frac{d}{dz}\Big(\chi' a_{,X_i}\nu\Big) \tag{1.12}
$$

for some λ independent of $i \in \{1, \dots, \mathcal{M}\}$ where $w_{,\phi_i}$ is evaluated at $\phi(z)$ and the derivatives of a at $(\phi(z), (e_\beta - e_\alpha) \otimes \nu)$.

Moreover, if ϕ is a solution to (1.9) then the surface energy is

$$
\sigma_{\alpha\beta}(\nu) = \frac{1}{3}\sqrt{a_{\alpha\beta}(\nu) w_{\alpha\beta}} \tag{1.13}
$$

Proof. Given ϕ as in (1.10) obviously $\phi(z) \to e_\beta \Leftrightarrow \chi(z) \to 1 \Leftrightarrow z \to \infty$ and $\phi(z) \to e_\alpha \Leftrightarrow \chi(z) \to 0 \Leftrightarrow z \to -\infty$ whence the second line of (1.8) follows. By assumption (1.4) $a_{,\phi}$ is two–homogeneous and $a_{,X}$ is one–homogeneous with respect to the second variable. Since $\partial_z\phi(z) \otimes \nu = \chi'(z)(e_\beta - e_\alpha)$

$$
\begin{aligned}
a_{,\phi}(\phi(z), \partial_z\phi(z) \otimes \nu) &= |\chi'(z)|^2 a_{,\phi}(\phi(z), (e_\beta - e_\alpha) \otimes \nu), \\
a_{,X}(\phi(z), \partial_z\phi(z) \otimes \nu) &= \chi'(z) a_{,X}(\phi(z), (e_\beta - e_\alpha) \otimes \nu).
\end{aligned}
$$

The first line of (1.8) then follows directly from (1.12).

A straightforward calculation shows the identities

$$
|\chi'|^2 = \frac{w_{\alpha\beta}}{a_{\alpha\beta}}\chi^2(1 - \chi)^2, \quad \chi'' = \frac{w_{\alpha\beta}}{a_{\alpha\beta}}\chi(1 - \chi)(1 - 2\chi). \tag{1.14}
$$

By assumption (1.5) $a(\phi(z), (e_\beta - e_\alpha) \otimes \nu) = a_{\alpha\beta}(\nu)$. Therefore, if ϕ solves (1.9) then the surface energy is (substituting $\frac{z}{2}\sqrt{\frac{a_{\alpha\beta}(\nu)}{w_{\alpha\beta}}} = t$)

$$\begin{aligned}
\sigma_{\alpha\beta}(\nu) &= \int_{\mathbb{R}} \Big(a(\phi, \partial_z \phi \otimes \nu) + w(\phi) \Big) dz \\
&= \int_{\mathbb{R}} \Big(|\chi'(z)|^2 a_{\alpha\beta}(\nu) + w_{\alpha\beta} \chi(z)^2 (1 - \chi(z))^2 \Big) dz \\
&= \int_{\mathbb{R}} 2 w_{\alpha\beta} (1 + \tanh(t))^2 (1 - \tanh(t))^2 \sqrt{\frac{a_{\alpha\beta}(\nu)}{w_{\alpha\beta}}} dt \\
&= \frac{1}{3} \sqrt{a_{\alpha\beta}(\nu) w_{\alpha\beta}}.
\end{aligned}$$

□

Now it is possible to state the aim precisely:

Task. *Construct admissible functions a and w such that*

1. *the values $\frac{1}{3}\sqrt{a_{\alpha\beta}(\nu) w_{\alpha\beta}}$ coincide with given surface energies $\sigma_{\alpha\beta}(\nu)$,*
2. *the function $\phi(z) = \chi(z) e_\beta + (1 - \chi(z)) e_\alpha$ with χ given by* (1.11) *fulfills condition* (1.12)*, and*
3. *this function $\phi(z)$ solves* (1.9)*.*

2. On the solvability of the task

In this section, an admissible gradient potential a will be presented which is based on the irreducible representations $\phi_\alpha \nabla \phi_\beta - \phi_\beta \nabla \phi_\alpha$ first used in [8] and later in [11] in the context of the phase field approach. Polynomial multi–well potentials w will also be presented such that the second point of the task set in the previous section is fulfilled and a critical point of the minimization problem (1.9) has the desired structure (1.10). In view of the first point, the values on the right hand side of (1.13) can be determined in terms of coefficients of a and w. In particular, the presented potentials allow for a large class of anisotropic surface energies $\sigma_{\alpha\beta}(\nu)$. It remains to examine whether the third point of the given task is satisfied. For this purpose, numerical simulations of test problems have been performed indicating when a critical point of the form (1.10) indeed solves the minimization problem (1.9). More results and other examples for gradient terms a and multi–well potentials w with the demanded properties including results of further numerical simulations will be published in a forthcoming paper [7].

Definition 2.1. For each $\alpha \neq \beta$, $\alpha, \beta \in \{1, \dots, \mathcal{M}\}$, let $s_{\alpha\beta} : \mathbb{R}^d \to \mathbb{R}$ be one–homogeneous functions which are positive on the unit sphere $S^{d-1} = \{\nu \in \mathbb{R}^d : \|\nu\|_2 = 1\}$, even and smooth (except in zero), and let $g_{\alpha\beta}$ positive coefficients. In addition the symmetries $g_{\alpha\beta} = g_{\beta\alpha}$ and $s_{\alpha\beta}(\nu) = s_{\beta\alpha}(\nu)$ for all $\nu \in S^{d-1}$,

$1 \le \alpha, \beta \le N$, are assumed to hold. The gradient potential in (1.2) is defined by

$$a(\phi, \nabla\phi) = \sum_{\alpha<\beta} g_{\alpha\beta}\big(s_{\alpha\beta}(\phi_\alpha \nabla\phi_\beta - \phi_\beta \nabla\phi_\alpha)\big)^2. \tag{2.1}$$

Observe that the homogeneity and the symmetry of the $s_{\alpha\beta}(\nu)$ yield $\nabla s_{\alpha\beta}(\nu)\cdot \nu = s_{\alpha\beta}(\nu)$ and $\nabla s_{\alpha\beta}(-\nu) = -\nabla s_{\alpha\beta}(\nu)$. Since

$$a(se_\beta + (1-s)e_\alpha), (e_\beta - e_\alpha)\otimes\nu) = g_{\alpha\beta}\big(s_{\alpha\beta}(\nu)\big)^2 = a_{\alpha\beta}(\nu) \tag{2.2}$$

is independent of $s \in [0,1]$ a fulfills the assumptions of Def. 1.1 and is admissible.

Proposition 2.2. *The multi–well potential*

$$w(\phi) = 9\sum_{\alpha<\beta} g_{\alpha\beta}\phi_\alpha^2\phi_\beta^2\Big(1 + 8\sum_{\delta\neq\alpha,\beta}\phi_\delta\Big) \tag{2.3}$$

satisfies the assumptions of Def. 1.1, and, given $a(\phi,\nabla\phi)$ by (2.1)*, the condition* (1.12) *of Lemma 1.2 is satisfied.*

Proof. It is easy to derive that (1.6) is fulfilled. Since $w(se_\beta + (1-s)e_\alpha) = 9g_{\alpha\beta}s^2(1-s)^2$ condition (1.7) is fulfilled, too, with $w_{\alpha\beta} = 9g_{\alpha\beta}$.

When evaluating the derivatives of a at $(\chi e_\beta + (1-\chi)e_\alpha, (e_\beta - e_\alpha)\otimes\nu)$ short calculations show that

$$\begin{aligned}
a_{,\phi_i} &= 2g_{\alpha\beta}(s_{\alpha\beta}(\nu))^2, \quad i = \alpha,\beta,\\
a_{,X_i} &= \begin{cases} 2g_{\alpha\beta}s_{\alpha\beta}(\nu)\nabla s_{\alpha\beta}(\nu)(-\chi), & i=\alpha,\\ 2g_{\alpha\beta}s_{\alpha\beta}(\nu)\nabla s_{\alpha\beta}(\nu)(1-\chi), & i=\beta,\end{cases}\\
\frac{d}{dz}\Big(a_{,X_i}\nu\chi'\Big) &= \begin{cases} 2g_{\alpha\beta}(s_{\alpha\beta}(\nu))^2(-\chi\chi'' - |\chi'|^2), & i=\alpha,\\ 2g_{\alpha\beta}(s_{\alpha\beta}(\nu))^2((1-\chi)\chi'' - |\chi'|^2), & i=\beta,\end{cases}
\end{aligned}$$

and if $i \neq \alpha,\beta$ it holds that $a_{,\phi_i} = 0$ and $a_{,X_i} = 0$, whence $\frac{d}{dz}(a_{,X_i}\nu\chi') = 0$. For the derivatives of w evaluated at $\phi = \chi e_\beta + (1-\chi)e_\alpha$ on can derive

$$w_{,\phi_i}(\chi e_\beta + (1-\chi)e_\alpha) = \begin{cases} 18g_{\alpha\beta}\chi^2(1-\chi), & i=\alpha,\\ 18g_{\alpha\beta}\chi(1-\chi)^2, & i=\beta,\\ 72g_{\alpha\beta}\chi^2(1-\chi)^2, & i\neq\alpha,\beta.\end{cases} \tag{2.4}$$

It follows then from (1.12) for $i \neq \alpha,\beta$ necessarily

$$\lambda = 72g_{\alpha\beta}\chi^2(1-\chi)^2 = 8w_{\alpha\beta}\chi^2(1-\chi)^2. \tag{2.5}$$

For $i = \alpha$ the right hand side of (1.12) reads using the identities (1.14) and (2.2)

$$\begin{aligned}
& w_{,\phi_\alpha} + |\chi'|^2 a_{,\phi_\alpha} - \frac{d}{dz}\Big(\chi' a_{,X_\alpha}\nu\Big)\\
= \;& 2w_{\alpha\beta}\chi^2(1-\chi) + \frac{w_{\alpha\beta}}{a_{\alpha\beta}(\nu)}\chi^2(1-\chi)^2\, 2a_{\alpha\beta}(\nu)\\
& - 2a_{\alpha\beta}(\nu)\Big(-\chi\frac{w_{\alpha\beta}}{a_{\alpha\beta}(\nu)}\chi(1-\chi)(1-2\chi) - \frac{w_{\alpha\beta}}{a_{\alpha\beta}(\nu)}\chi^2(1-\chi)^2\Big)
\end{aligned}$$

$$\begin{aligned} &= 2w_{\alpha\beta}\chi^2(1-\chi) + w_{\alpha\beta}\chi^2(1-\chi)^2 \\ &\quad + w_{\alpha\beta}(\nu)\Big(4\chi^2(1-\chi)^2 - 2\chi^2(1-\chi) + 2\chi^2(1-\chi)^2\Big) \\ &= 8w_{\alpha\beta}\chi^2(1-\chi)^2 \quad = \quad \lambda, \end{aligned}$$

hence condition (1.12) holds for $i = \alpha$ with λ given by (2.5). Similarly this can be shown for $i = \beta$. □

Theorem 2.3. *The multi-well potential*

$$w(\phi) = 9\sum_{\alpha<\beta} g_{\alpha\beta}\phi_\alpha^2\phi_\beta^2\Big(1 + 8\sum_{\delta\neq\alpha,\beta}\phi_\delta\Big) + \sum_{\alpha<\beta<\delta} g_{\alpha\beta\delta}\phi_\alpha^2\phi_\beta^2\phi_\delta^2 \tag{2.6}$$

satisfies the assumptions of Def. 1.1. Given $a(\phi, \nabla\phi)$ by (2.1) *the second point of the set task is satisfied.*

Proof. For the additional term $w_{add}(\phi) := \sum_{\alpha<\beta<\delta} g_{\alpha\beta\delta}\phi_\alpha^2\phi_\beta^2\phi_\delta^2$ it holds that $(w_{add})_{,\phi}(\chi e_\beta + (1-\chi)e_\alpha) = 0$. Therefore, (2.4) is not changed. Hence, the same arguments as in the proof of the preceding proposition followed by Lemma 1.2 can be applied to show the theorem. □

Observe that $a_{\alpha\beta}(\nu) = g_{\alpha\beta}(s_{\alpha\beta}(\nu))^2$ and $w_{\alpha\beta} = 9g_{\alpha\beta}$ yield

$$\sigma_{\alpha\beta}(\nu) = g_{\alpha\beta}s_{\alpha\beta}(\nu)$$

from Lemma 1.2 if, in addition, also the third point of the given task is satisfied. In order to recover a prescribed surface energy the idea is that $g_{\alpha\beta}$ determines its typical size involving the physical units (one may choose the mean value of $\sigma_{\alpha\beta}(\nu)$ on the unit sphere) and that $s_{\alpha\beta}(\nu)$, a dimensionless multiplier, models the deviations from this typical value depending on the direction ν, i.e., the anisotropy. In spite of the constraints imposed on the $g_{\alpha\beta}$ and the $s_{\alpha\beta}(\nu)$ in Def. 2.1 a wide class of anisotropic surface tensions can be recovered by that procedure. Hence, there is a good chance that the first point of the set task can be fulfilled provided the third point is satisfied for the presented potentials. Numerical experiments for test problems have been performed and are presented in the following section indicating that this is in fact the case.

3. Numerical tests

In the following let $\alpha = 1$ and $\beta = 2$. In one space dimension a sharp transition relaxed under a gradient flow of the energy (1.2) (cp. (4.1) in the following section), i.e., a jump of ϕ from e_1 to e_2, expecting a stable form which approximates a solution to (1.9). Let $M = 3$, $\varepsilon = 0.1$ and consider the domain $D = [0, 1]$ discretized with a uniform grid of mesh size $\Delta x = 0.01$. Homogeneous boundary conditions were imposed which were checked to have no influence on the results. For the numerical method based on finite differences [6] is an appropriate reference.

Choosing $g_{\alpha\beta} = 1$ and $s_{\alpha\beta}(\nu) = 1$ for all pairs (α, β), very small contributions of the order 10^{-4} of phase 3 in the transition region were found after relaxation.

Refining the grid, the contributions became even smaller indicating that discretization errors had come in. Also the case of different surface energies was examined defining g_{12}, g_{13} and g_{23} by a permutation of the values $\frac{2}{\sqrt{3}}$, 1.0 and $\frac{1}{\sqrt{3}}$. If $g_{12} = \frac{2}{\sqrt{3}}$ the largest contributions from phase 3 of order 10^{-3} were observed. As in the case of equal surface energies they became smaller when refining the grid.

For $M = 4$ the multi–well potential (2.3) converges to $-\infty$ if $\xi \to \infty$ and $\phi = \xi(1, 1, -1, -1)$. During the relaxation of the sharp phase transition it was indeed observed that ϕ_3 and ϕ_4 were equal and grew such that no equilibrium was reached. Adding a coercive term as in (2.6) the blow up could be avoided. Analogously, if $M > 4$ the additional term in w turned out to be necessary.

Let $g_{\alpha\beta} = 1$ and $s_{\alpha\beta}(\nu) = 1$ as before and use the potential (2.6) where $g_{\alpha\beta\delta} = C$ for all triples α, β, δ with a positive constant C. In the case $M = 4$, for $C \leq 120.0$ we found large contributions of the phases 3 and 4 of order 10^{-1} in the transition region. The energy (1.2) can be approximated by the sum

$$\mathcal{F}_{approx} := \Delta x \sum_{i=0}^{N} \varepsilon\, a(\phi(x_i), \partial_x^h \phi(x_i)) + \frac{1}{\varepsilon} w(\phi(x_i)),$$

where $\partial_x^h \phi(x_i) = \frac{1}{\Delta x}(\phi(x_{i+1}) - \phi(x_i))$ and the $\{x_i\}_{i=0}^N$ are the grid points. Computing this sum gives energies of $\mathcal{F}_{approx} = 0.970590$ if $C = 5.0$, i.e. in the presence of third phase contributions, and $\mathcal{F}_{approx} = 0.999242$ if $C = 200.0$ without. This indicates that if C is to small then the solution to (1.9) has not the form (1.10). Moreover, the approximation of the surface energy, here $\sigma_{\alpha\beta}(\nu) = 1$, is worse in that case.

To examine whether a given surface energy is correctly recovered by the phase field model the contraction of a sphere by a curvature flow in two space dimensions is a good test problem since an analytical solution is known. Using matched asymptotic expansions, it is shown in [5] that the phase field model yields a model with free boundaries moving according to a curvature flow in the sharp interface limit as $\varepsilon \to 0$. For a sphere in 2D, this curvature flow can be expressed in terms of the radius $r(t)$ being a function of the time t and reads

$$\dot{r}(t) = -\frac{\sigma}{r(t)}, \quad r(0) = r_0. \tag{3.1}$$

For $\sigma = 1$ the exact solution is $r(t) = \sqrt{r_0^2 - 2t}$.

On the domain $D = [0, 2]^2$ phase 1 initially occupied a quarter of a ball with radius $r_0 = 1.4$ centered in $(0, 0)$, phase 2 occupied the remaining part of D, and another phase 3 is considered but initially nowhere present. The initial data were chosen as follows:

$$\phi_{1,ic} = \tfrac{1}{2}\big(1 - \tanh(\tfrac{3(r-r_0)}{2\varepsilon})\big), \quad \phi_{2,ic} = 1 - \phi_{1,ic}, \quad \phi_{3,ic} = 0.$$

The other parameters were $\varepsilon = 0.2$, $\Delta x = 0.01$, $g_{\alpha\beta} = 1$ and $s_{\alpha\beta}(\nu) = 1$ for all pairs $\alpha < \beta$. Homogeneous Neumann boundary conditions were imposed. Two numerical simulations were performed, a first one with the straightforward generalization

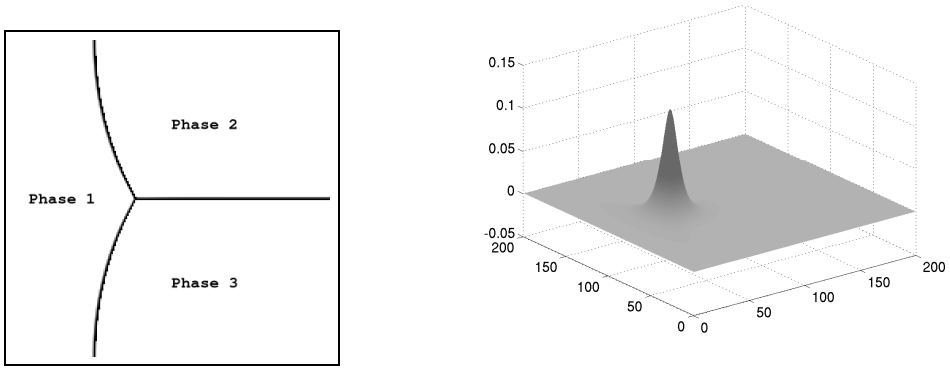
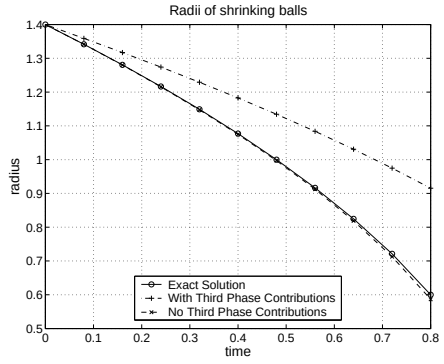


FIGURE 1. On the left: Simulated triple junction. On the right: Contribution of phase 4 in the triple junction.

$w(\phi) = 9\sum_{\alpha<\beta} g_{\alpha\beta}\phi_\alpha^2\phi_\beta^2$ of the standard multi–well potential and a second one with the new potential (2.3).



During the first simulation a strong contribution of ϕ_3 in the interfacial layer was observed in contrast to the second simulation. The figure shows the radii of the sets where $\phi_1 = \phi_2$ in comparison with the exact solution over the time. If no third phase contributions are present the simulation approximates remarkably good the exact solution while in the other case the velocity of the shrinking circle is too small. This is consistent with the results in [6]. There for the above choice of w a surface energy $\sigma < 1$ was measured which, by (3.1), leads to a slower motion.

When simulating with $\mathcal{M} = 4$ or more phases, phase field variables are present in the region of a triple junction which do not correspond to the adjacent phases. Fig. 1 shows a triple junction on the domain $D = [0,1]^2$. Thanks to an appropriate choice of the $g_{\alpha\beta\delta}$, on the phase transitions no contributions of other phase field variables than corresponding to the adjacent phases are observed. But in the triple junction a fourth phase has developed which was not present initially ($\phi_4(t = 0) = 0$) and whose height turned out to be independent of ε and Δx. Nevertheless, the angles in the triple point still agree remarkably well with the theoretically predicted values of 120° (see [3]) in spite of the presence of the artificial fourth order contributions.

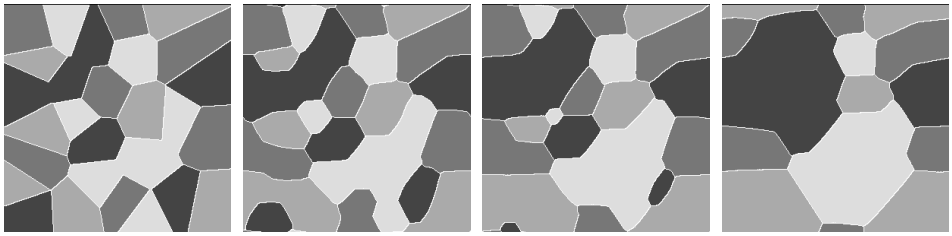


FIGURE 2. Growth of grains. From left to right and from top to bottom the situation at the times t =0.0, 0.0036, 0.0108, and 0.9.

4. Applications

As a first application example grain growth involving four grains of different structure was simulated, modeled by a L^2–gradient flow of the energy (1.2). It reads

$$\omega\partial_t\phi_\alpha = \varepsilon\big(\nabla\cdot a_{,X_\alpha}(\phi,\nabla\phi) - a_{,\phi_\alpha}(\phi,\nabla\phi)\big) - w_{,\phi_\alpha} - \lambda \tag{4.1}$$

with an appropriate Lagrange multiplier λ ensuring $\partial_t\phi \in T\Sigma^{\mathcal{M}}$ and a calibration constant ω. For the surface energy anisotropies the crystalline functions

$$s_{\alpha\beta}(\nu) = \max\{\eta_{\alpha\beta}^{(k)}\cdot\nu,\, k=1,\dots,6\},$$

were chosen where the $\{\eta_{\alpha\beta}^{(k)}\}_k$ are the edges of a hexagonal crystal. For every phase transition the same surface energy was chosen, namely $g_{\alpha\beta}=1$ and

$$\left\{\eta_{\alpha\beta}^{(k)}\right\}_{k=1}^{6} = \left\{ \binom{1}{0}, \frac{1}{2}\binom{1}{\sqrt{3}}, \frac{1}{2}\binom{-1}{\sqrt{3}}, \binom{-1}{0}, \frac{1}{2}\binom{-1}{-\sqrt{3}}, \frac{1}{2}\binom{1}{-\sqrt{3}} \right\}$$

for all $\alpha<\beta$. On the domain $D=[0,1]^2$ the system of parabolic partial differential equations (4.1) was discretized explicitly in time using a finite difference method (gradients were replaced by forward differences, the divergence by a backward difference, cp. [6]). The values for the phase field variables were initialized using a Voronoj diagram. The grid size of the uniform grid was $\Delta x = 0.0033$, the time step $\Delta t = 1.5\cdot 10^{-6}$. Setting $g_{\alpha\beta\delta}=250.0$ for all triples $\alpha<\beta<\delta$ third phase contributions on the phase boundaries could be avoided. Periodic boundary conditions were imposed. Fig. 2 shows the evolution of the grains. During the relaxation, the angles remarkably good approximate the predicted values of 120° and the phase boundaries are oriented according to the preferred directions (cp. [1] for the crystalline curvature flow resulting from the gradient flow of (1.1) with such crystalline surface energies).

As a second example the gradient flow (4.1) for three phases (two solid phases and liquid one) was coupled to parabolic evolution equations balancing the mass respectively the concentrations of two components of a eutectic alloy (cp. [4] for a description of a general model for solidification of alloys on which the present one is based). The concentrations are denoted by c_1 and c_2 and satisfy the algebraic

constraint $c_1 + c_2 = 1$ and the partial differential equations

$$\partial_t c_i = -\nabla \cdot J_i = -\nabla \cdot \sum_{j=1}^{2} L_{ij} \nabla \frac{-\mu_j}{T}, \quad 1 \leq i \leq 2.$$

The J_i are the fluxes and satisfy $J_1 + J_2 = 0$ for that the algebraic constraint remains fulfilled during the evolution. The Onsager coefficients L_{ij} constitute a symmetric matrix and were chosen to be

$$L_{11} = L_{22} = -L_{12} = -L_{21} = D^{(\alpha)} c_i (1 - c_i)$$

with diffusion coefficients D^α depending on the phase but independent of the components. In the liquid phase D^α was set to 1.5 while in the two solid phases to 0.015. The chemical potentials μ_j are the derivatives of the free energies of the possible phases with respect to the concentrations, $\mu_j = \partial_{c_j} f$. The free energies were chosen of the form

$$f^\alpha(c, \phi) := \sum_{\alpha=1}^{3} \sum_{i=1}^{2} \left(c_i L_i^\alpha \frac{T - T_i^\alpha}{T_i^\alpha} h(\phi_\alpha) \right) + \sum_{i=1}^{2} T c_i \ln(c_i).$$

The function h satisfying $h(0) = 0$ and $h(1) = 1$ is an interpolation function. The quantity L_i^α is the latent heats per unit volume of the phase transition from phase α to the liquid phase and of the pure component i, and T_i^α is the melting temperature of the i-th component in phase α. Indexing the solid phases with α and β and the liquid one with l the following values were chosen:

$$L_i^\alpha = L_i^\beta = 10.5467,\ L_i^l = 0,\ \forall i, \quad T_1^\alpha = T_2^\beta = 2.4,\ T_2^\alpha = T_1^\beta = 1.6.$$

These choices yield a symmetric eutectic phase diagram with a eutectic concentration of $c_E = 0.5$, a eutectic temperature of about $T_E \approx 2.11686$, and equilibrium concentrations $c^\alpha = 0.1$ and $c^\beta = 0.9$ of the solid phases at eutectic temperature. The above choice of the Onsager coefficients together with this free energy density yields linear diffusion equations in the pure phases, cp. [4].

The system temperature T was kept constant during the simulation and set to 2.01686 which means that the liquid is slightly undercooled. The evolution of the phase field variables is coupled to the thermodynamic quantities be adding a term $-\frac{1}{T} f_{,\phi_\alpha}(c, \phi)$ to the right hand side of (4.1). The remaining values were set to $\varepsilon = 0.4$ and $\omega = 0.1$. Initially, a situation as in Fig. 3 on the left was considered on the domain $[4.8, 9.6]$. The concentrations in the phases were chosen according to the equilibrium values at eutectic temperature. To the left and to the right periodic boundary conditions were imposed while to the top and to the bottom homogeneous Neumann boundary conditions. The initial situation relaxed on a uniform grid with spacing $\Delta x = 0.04$ and time stepping $\Delta t = 0.0002$. After a while, a self–similar lamellar growth of the solid phases into the liquid one was observed (see Fig. 3). For more numerical simulations and results on eutectic alloys [9] is an appropriate reference.

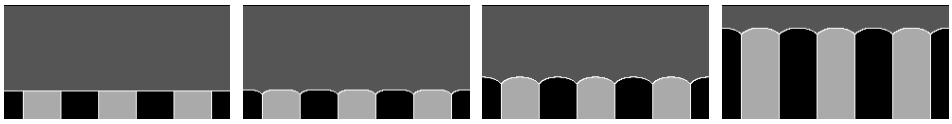


FIGURE 3. Eutectic solidification, lamellar solid structure growing self–similarly (after a while) into an undercooled melt. From the left to the right the situation at $t = 0.0, 0.06, 1.2, 6.0$.

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