A Semi discretization Scheme
for a phase-field model of a binary alloy

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Abstract: *The aim of this paper is to show the existence of solutions to a nonlinear problem arising from the isothermal solidification of a binary alloy in two dimensional domain. For this, a mathematical analysis of a time discretization scheme is considered. We establish a discrete maximum principle to obtain the a priori estimates. The convergence of the solutions of discrete scheme is proved and existence and regularity results for the original problem are derived.*

1 Introduction

Phase separation observed during the solidification process of materials is an important and fascinating topic for researches. It is a difficult topic, though, and one of the principal obstacles in predicting solidification patterns is the difficulty of accurately calculating the processes occurring in the liquid and solid regions for the complex shapes of the liquid-solid interfaces that appear during the process. For the treatment of the such interfaces, the phase-field method has emerged as a powerful tool, among the large class of the methods that rely on treating a macroscopically sharp interface as a diffuse region. In this type of modeling, an extra variable, the so called phase-field $\varphi(x,t)$, is introduced as an order parameter used to describe the phases of the material. The behavior of this variable is governed by a suitable equation that is then coupled to other equations obtained by the more usual balancing of mass, momentum, energy or solute, according the peculiar situation under investigation. Therefore, it is important to understand the mathematical problems resulting from this approach.

Following this line of research, the goal of this paper is to analyze a nonlinear parabolic system of highly nonlinear partial differential equations arising by using this kind of modeling in a isothermal solidification process of a binary alloy. More precisely, we consider a phase-field model motivated by the ones in [1, 2, 4, 11]. In the model to be analyzed, the state of the alloy is characterized by the relative concentration c (the proportion of solute in the solvent) and phase-field φ. When $\varphi = 0$ the alloy is considered to be liquid, $\varphi = 1$ the alloy is solid. The region when $0 < \varphi < 1$ corresponds to the solid-liquid transition region, which is sometimes called the mushy region.

Let $\Omega \subset \mathbb{R}^2$ be an open bounded domain with a C^2 boundary and $Q = \Omega \times (0,T)$ the space-time cylinder with lateral surface $S = \partial\Omega \times (0,T)$. Then, we consider the following nonlinear system **(P)**:

$$\partial_t \varphi - \xi^2 \Delta\varphi = \varphi(\varphi-1)(1-2\varphi) - |\nabla\varphi|\, c \ \text{ in } Q,$$
$$\partial_t c - \mathrm{div}(D_1(\varphi)\nabla c) = \mathrm{div}(D_2(c,\varphi)\nabla\varphi) \ \ \text{ in } Q,$$
$$\varphi = 0, \quad c = 0 \ \text{ on } \ S,$$
$$\varphi(x,0) = \varphi_0(x), \quad c(x,0) = c_0(x) \ \text{ in } \ \Omega,$$

Here, ξ is a positive constant associated to material properties; $D_1(\cdot)$ and $D_2(\cdot)$ are diffusion coefficients of the solute in the matrix of the solvent, that is, the other material constituting the binary alloy; $\varphi_0(\cdot)$ and $c_0(\cdot)$ are the ini-

tial conditions respectively for the phase-field and solute concentration. For simplicity of exposition, we assumed homogeneous Dirichlet boundary conditions; with simple modifications of the arguments, similar analysis could be done for other kinds of boundary conditions; for instance, we could take homogeneous Neumann boundary conditions for some of all of the unknown; consider appropriate nonhomogeneous boundary conditions, and so on.

The previous phase-field equation was derived by Beckermann, Diepers, Steinbach in [1], but here it is presented in a form obtained there before a final simplification was carried out. Thus, in a certain sense the phase field equation given in **(P)** can be considered more accurate than the final form stated in [1]. The concentration equation is obtained by rather general forms of balances of mass and generalize the cases of [1, 4, 11].

In this paper, an existence result for solutions will be obtained for the case of two-dimensional domain by using a time discretization scheme to construct approximate solutions. Regularity and uniqueness will be obtained when $D_1(\varphi)$ and $D_2(c, \varphi)$, and the other data are smooth enough.

The outline of the paper is the following. The next section is dedicated to fix the notations, to introduce the basic functional spaces to be used, to collect some results about interpolation inequalities and embeddings, as well as to explicitly describe our general assumptions. Also in this section, we introduce the time-discretization scheme to be used and state the main results of the paper. In Section 3 contains the proof of the existence of the discrete solution, that is, solutions of the corresponding discretized scheme, as well as certain results on their regularity. In Section 4 we establish a discrete maximum principle for the semi discrete problem related to the phase field equation. This result is important to obtain the *a priori* estimates of semi discrete scheme and it is only proved for the case of two-dimensional.. Existence of a weak solution is proved in Section 5 by using a collection of estimates, uniform with respect to the time-discretization step. In Section 6 presents further regularity and uniqueness of the solutions.

Finally, we remark that, as usual in this kind of context, throughout the article we will denote by M, and sometimes $M_1, M_2, \ldots$, constants depending only on known quantities.

2 Notation, assumptions and auxiliary results

We denote the Banach space $W_q^{2,1}(Q)$ consists of functions $u(x,t)$ in $L^q(Q)$ whose generalized derivatives $\partial_x u$, $\partial_x^2 u$, $\partial_t u$ are L^q-integrable; here ∂_x^s denotes all the partial derivatives with respect to $x_1, \ldots, x_n$ of order s. Its norm is given by

$$||u||_{q,Q}^{(2)} = ||u||_{q,Q} + ||\partial_x u||_{q,Q} + ||\partial_x^2 u||_{q,Q} + ||\partial_t u||_{q,Q}.$$

We refer to [5, 8], for instance, for more details of the previous spaces.

We will also need the following Gagliardo-Nirenberg type interpolation inequalities stated in the following lemmas (see Zheng [13, p. 3]):

Lemma 2.1 *Let $\Omega \subset \mathbb{R}^d$, $d = 1$, 2 or 3, is a bounded domain with a C^2-boundary. Then, there exist a positive constant M such that*

$$||\nabla u||_{4,\Omega}^2 \leq M ||\Delta u||_{2,\Omega} \, ||u||_{\infty,\Omega}, \qquad (2.1)$$

$\forall \, u \in H_0^2(\Omega) \cap L^\infty(\Omega).$

In lower dimensions, the following holds:

Lemma 2.2 *Let $\Omega \subset \mathbb{R}^d$, $d = 1$ or 2 is a bounded domain with a C^2-boundary. Then, there exist a positive constant M such that*

$$||u||_{4,\Omega}^2 \leq M ||u||_{2,\Omega} \, ||\nabla u||_{2,\Omega}, \qquad (2.2)$$

$\forall \, u \in H_0^1(\Omega) \cap L^2(\Omega).$

$$||\nabla u||_{4,\Omega}^2 \leq M ||\nabla u||_{2,\Omega} \, ||\Delta u||_{2,\Omega}, \qquad (2.3)$$

$\forall \, u \in H_0^2(\Omega) \cap H^1(\Omega).$

Throughout this paper we shall make the following assumptions:

(H): $\Omega \subset \mathbb{R}^2$ is a bounded domain with C^2-boundary;

$D_1(\cdot) \in C^0(\mathbb{R})$ such that
$$0 < \rho_0 \leq D_1(\cdot) \leq \rho_1, \; \rho_0, \rho_1 \in \mathbb{R}^+;$$

$D_2(\cdot, \cdot) \in C^0(\mathbb{R}^2)$ such that
$$|D_2(\cdot, \cdot)| \leq \alpha_0, \; \alpha_0 \in \mathbb{R}^+.$$

In this paper we shall frequently make use of some auxiliary results, which we list below for further reference.

Frequently we shall use the discrete Gronwall Lemma:

Lemma 2.3 *Let τ, M, u_n, v_n (for intergers $n \geq 0$) be nonnegative numbers such that*

$$u_n \leq M + \tau \sum_{k=0}^{n} v_k\, u_k \quad \text{for} \ \ n \geq 0.$$

Suppose that $\tau v_k < 1$. Then

$$u_n \leq M\, exp\left(\tau \sum_{k=0}^{n} \frac{v_k}{1 - \tau v_k}\right) \quad \text{for} \ \ n \geq 0.$$

At various places we shall use the following relation

$$2 \int_{\Omega} a(a - b)\, dx = ||a||_{2,\Omega}^2 - ||b||_{2,\Omega}^2 + ||a - b||_{2,\Omega}^2. \tag{2.4}$$

Our next lemma provides a compactness criterion:

Lemma 2.4 *Let X and Y be two (not necessarity reflexive) Banach spaces, such that $Y \subset X$, the injection being compact.*

Assume that $\mathcal{G}$ is a family of functions in $L^1(0, T; Y) \cap L^p(0, T; X)$ for some $T > 0$ and $p > 1$, such that

$$\mathcal{G} \text{ is bounded in } L^1(0,T;Y) \text{ and } L^p(0,T;X); \tag{2.5}$$

$$\sup_{g \in \mathcal{G}} \int_0^{T-a} ||g(a+s) - g(s)||_X^p\, ds \to 0 \tag{2.6}$$
$$\text{as} \ \ a \to 0, \ \ a > 0.$$

Then the family $\mathcal{G}$ is relatively compact in $L^p(0,T;X)$.

2.1 Semi discretization

We consider a semi discretization of problem **(P)** with respect to the time variable as follows: we subdivide $[0, T]$ into N subintervals $[t_{m-1}, t_m]$, $t_m = \tau\, m$, $\tau = T/N$, and for $m = 1, 2, \cdots, N$ we consider the following system of elliptic problems **(PD)**:

$$\delta_t \varphi^m - \xi^2 \Delta \varphi^m = (\varphi^{m-1} - 1)(1 - 2\varphi^{m-1})\varphi^m$$
$$-|\nabla \varphi^m|\, c^{m-1} \quad \text{a.e. in} \ \ \Omega,$$
$$\delta_t c^m - \text{div}(D_1(\varphi^m)\nabla c^m) =$$
$$\text{div}(D_2(c^m, \varphi^m)\nabla \varphi^m) \quad \text{a.e. in} \ \Omega,$$
$$\varphi^m = 0, \ \ c^m = 0 \ \text{ a.e. in} \ \ \partial\Omega,$$

where $\varphi^0 = \varphi_0(x)$, $c^0 = c_0(x)$, $\delta_t \varphi^m = (\varphi^m - \varphi^{m-1})/\tau$, $\delta_t c^m = (c^m - c^{m-1})/\tau$ and φ^m and c^m, $m = 1, ..., N$, are expected to be approximations of $\varphi(x, t_m)$ and $c(x, t_m)$, respectively.

We will prove the following existence result for discrete scheme **(PD)**:

Theorem 2.1 *There exists an unique solution (φ^m, c^m) in $H^2(\Omega) \times H_0^1(\Omega)$ of the approximate problem **(PD)**.*

With this result we may introduce the functions: for $t \in [t_{m-1}, t_m]$, and $1 \leq m \leq N$, we define $\widetilde{\varphi}_\tau(t) = \varphi^{m-1} + (t - t_{m-1})\delta_t \varphi^m$, $\widetilde{c}_\tau(t) = c^{m-1} + (t - t_{m-1})\delta_t c^m$, and corresponding step functions are given by $\varphi_\tau(t) = \varphi^m$ and $c_\tau(t) = c^m$.

The sequence of functions $(\widetilde{\varphi}_\tau, \widetilde{c}_\tau)$ can be expected to converge as $\tau \to 0$, in suitable function spaces. The limit function (φ, c) is expected to be a solution to the problem **(P)**:

Theorem 2.2 *Assume that **(H)** holds. Suppose $(\varphi_0, c_0) \in H^1(\Omega) \cap L^2(\Omega)$ with $0 \leq \varphi_0(x) \leq 1$ for a.e. $x \in \Omega$. Then there exists functions (φ, c) satisfying $(\varphi, c) \in W_2^{2,1}(Q) \times (L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H_0^1(\Omega)))$ and $c_t \in L^2(0, T; H^{-1}(\Omega))$, such that $(\varphi(0), c(0)) = (\varphi_0, c_0)$ and*

$$\langle c_t, v \rangle + \int_{\Omega} D_1(\varphi)\nabla c \nabla v\, dx =$$
$$-\int_{\Omega} D_2(\varphi, c)\nabla \varphi\, \nabla v\, dx,$$

for all $v \in H_0^1(\Omega)$ a.e. in $(0, T)$,

$$\varphi_t - \xi^2 \Delta \varphi = \varphi(\varphi - 1)(1 - 2\varphi) - |\nabla \varphi|\, c \ \ \text{in} \ Q,$$
$$\varphi = 0 \ \ \text{on} \ S.$$

When c_0, D_1 and D_2 are smooth enough, we may have further regularity properties:

Theorem 2.3 *Assume that **(H)** holds. Suppose $c_0 \in H_0^1(\Omega)$, $D_1(\varphi)$ and $D_2(c, \varphi,)$ are differentiable, with $\nabla D_1 \in L^\infty(\mathbb{R})$ and $\nabla D_2 \in L^\infty(\mathbb{R}^2)$. Then there exists an unique solution $(\varphi, c) \in (W_2^{2,1}(Q))^2$ of the problem **(P)**.*

3 Proof of Theorema 2.1

For a fixed m, assuming that φ^{m-1} and c^{m-1} are already known and we consider the following nonlinear system:

$$-\tau \xi^2 \Delta \varphi^m + \varphi^m = \tau\, (\varphi^{m-1})(1 - 2\varphi^{m-1})\varphi^m -$$
$$\tau |\nabla \varphi^m|\, c^{m-1} + \varphi^{m-1} \quad \text{in} \ \ \Omega,$$

$$-\tau \, \text{div}(D_1(\varphi^m)\nabla c^m) + c^m =$$
$$\tau \text{div}(D_2(c^m, \varphi^m)\nabla \varphi^m) + c^{m-1} \quad \text{in} \ \ \Omega,$$

$$\varphi^m = 0, \ \ c^m = 0 \quad \text{on} \ \ \partial\Omega.$$

The proof the Theorem 2.1 will be omitted.

4 Discrete maximum principle

Next, we establish a discrete maximum principle for the semi discrete problem:

$$\delta_t \varphi^m - \xi^2 \Delta \varphi^m = (\varphi^{m-1} - 1)(1 - 2\varphi^{m-1})\varphi^m -$$

$$|\nabla \varphi^m| \, c^{m-1} \quad \text{a.e. in} \quad \Omega, \qquad (4.7)$$

$$\varphi^m = 0 \quad \text{a.e. on} \quad \partial\Omega.$$

where $\varphi^0 = \varphi_0(x)$ such that $0 \le \varphi_0(x) \le 1$ and $\delta_t \varphi^m = (\varphi^m - \varphi^{m-1})/\tau$.

Now, we multiplying the equation (4.7) by $2\tau\varphi_-^m$, integrating over Ω and using Green's formula, we obtain

$$2\int_\Omega (\varphi^m - \varphi^{m-1})\varphi_-^m \, dx + 2\tau\xi^2 \int_\Omega |\nabla\varphi_-^m|^2 \, dx =$$

$$2\tau \int_\Omega (\varphi^{m-1} - 1)(1 - 2\varphi^{m-1})(\varphi_-^m)^2 \, dx -$$

$$2\tau \int_\Omega |\nabla\varphi_-^m| c^{m-1} \varphi_-^m \, dx.$$

Moreover, we can write

$$2\int_\Omega (\varphi_-^m - \varphi_-^{m-1})\varphi_-^m \, dx +$$

$$2\int_\Omega (\varphi_-^{m-1} - \varphi^{m-1})\varphi_-^m \, dx + 2\tau\xi^2 \int_\Omega |\nabla\varphi_-^m|^2 \, dx =$$

$$2\tau \int_\Omega (\varphi^{m-1} - 1)(1 - 2\varphi^{m-1})(\varphi_-^m)^2 \, dx -$$

$$2\tau \int_\Omega |\nabla\varphi_-^m| c^{m-1} \varphi_-^m \, dx.$$

Now, using that $2\displaystyle\int_\Omega (\varphi_-^{m-1} - \varphi^{m-1})\varphi_-^m \, dx \ge 0$, $\max_{s \in \mathbb{R}}(s-1)(1-2s)$ is finite, and Hölder's and Young's inequalities, we get

$$2\int_\Omega (\varphi_-^m - \varphi_-^{m-1})\varphi_-^m \, dx + 2\tau\xi^2 ||\nabla\varphi_-^m||_{2,\Omega}^2 \le$$

$$\tau M_1 ||\varphi_-^m||_{2,\Omega}^2 + \tau ||\nabla\varphi_-^m||_{2,\Omega} ||c^{m-1}||_{4,\Omega} ||\varphi_-^m||_{4,\Omega}.$$

Using the relation (2.4) and Young's inequality, we obtain

$$||\varphi_-^m||_{2,\Omega}^2 - ||\varphi_-^{m-1}||_{2,\Omega}^2 + ||\varphi_-^m - \varphi_-^{m-1}||_{2,\Omega}^2 +$$

$$\tau\xi^2 ||\nabla\varphi_-^m||_{2,\Omega}^2 \le$$

$$\tau M_1 ||\varphi_-^m||_{2,\Omega}^2 + \frac{\tau}{\xi^2} ||c^{m-1}||_{4,\Omega}^2 ||\varphi_-^m||_{4,\Omega}^2.$$

Using the result interpolation (2.2) and Young's inequality, we have

$$||\varphi_-^m||_{2,\Omega}^2 - ||\varphi_-^{m-1}||_{2,\Omega}^2 +$$

$$||\varphi_-^m - \varphi_-^{m-1}||_{2,\Omega}^2 + \frac{\tau\xi^2}{2} ||\nabla\varphi_-^m||_{2,\Omega}^2 \le$$

$$\tau M_1 ||\varphi_-^m||_{2,\Omega}^2 + \frac{\tau}{2\xi^6} ||c^{m-1}||_{4,\Omega}^4 ||\varphi_-^m||_{2,\Omega}^2.$$

Summing these relations for $m = 1, 2, ..., r$, with $1 \le r \le N$, we find

$$||\varphi_-^r||_{2,\Omega}^2 + \sum_{m=1}^r ||\varphi_-^m - \varphi_-^{m-1}||_{2,\Omega}^2 +$$

$$\frac{\tau\xi^2}{2} \sum_{m=1}^r ||\nabla\varphi_-^m||_{2,\Omega}^2 \le$$

$$||\varphi_-^0||_{2,\Omega}^2 + \tau \sum_{m=1}^r \left(M_1 + \frac{1}{2\xi^6} ||c^{m-1}||_{4,\Omega}^4 \right) ||\varphi^m||_{2,\Omega}^2$$

From discrete Gronwall Lemma 2.3

$$||\varphi_-^r||_{2,\Omega}^2 \le$$

$$M_2 ||\varphi_-^0||_{2,\Omega}^2 \exp\left(\tau \sum_{m=1}^r \frac{1}{2\xi^6} ||c^{m-1}||_{4,\Omega}^4 \right).$$

Since $\varphi_-^0 = 0$, we conclude that $||\varphi_-^r||_2^2 = 0$. Hence $\varphi_-^m = 0$ for all m and a.e. in Ω.

In the same way, $\varphi^0 \le 1$ a.e in Ω implies that $\varphi^m \le 1$ for all m and a.e. in Ω; it is sufficient to multiply the equation (4.7) by $(1-\varphi^m)_-$ and proceed similarity as before.

Then, we proved that

$$0 \le \varphi^m(x) \le 1, \quad \forall m, \text{ a.e. in } \Omega. \qquad (4.8)$$

5 Proof of Theorem 2.2

Lemma 5.1 *For τ sufficiently small the following estimates are satisfied:*

$$||(\varphi_\tau, \widetilde{\varphi}_\tau)||_{(L^\infty(0,T;H^1(\Omega)))^2} \le M,$$

$$||(\varphi_\tau, \widetilde{\varphi}_\tau)||_{L^2(0,T;H^2(\Omega))^2} \le M,$$

$$||(c_\tau, \widetilde{c}_\tau)||_{(L^\infty(0,T;L^2(\Omega)))^2} \le M,$$

$$||(c_\tau, \widetilde{c}_\tau)||_{L^2(0,T;H^1(\Omega)))^2} \le M,$$

$$||\partial_t \widetilde{\varphi}_\tau||_{2,Q} \le M.$$

Moreover, $||(\widetilde{\varphi}_\tau - \varphi_\tau, \widetilde{c}_\tau - c_\tau)||_{(L^2(Q))^2} \le \tau M.$

The proof the Theorem 2.1 will be omitted.

5.1 Taking the limit

We deduce from Lemma 5.1 that $(\widetilde{\varphi}_\tau, \varphi_\tau)$, $(\widetilde{c}_\tau, c_\tau)$ are bounded (uniformly with respect to τ) in $W_2^{2,1}(Q) \times L^2(0,T;H^2(\Omega))$ and $(L^2(0,T;H_0^1(\Omega)))^2$, respectively. Moreover, $W_2^{2,1}(Q)$ is compactly embedding into $L^p(Q)$ with $1 \le p < \infty$ (see [9]). Hence, there exist $(\widetilde{\varphi}, \varphi) \in W_2^{2,1}(Q) \times L^2(0,T;H^2(\Omega))$, $(\widetilde{c}, c) \in (L^2(0,T;H_0^1(\Omega)))^2$ and subsequences still denote (φ_τ, c_τ), $(\widetilde{\varphi}_\tau, \widetilde{c}_\tau)$, such that as $\tau \to 0$,

$$
\begin{aligned}
\widetilde{\varphi}_\tau &\rightharpoonup \widetilde{\varphi} \ \text{ in } \ W_2^{2,1}(Q), \\
\varphi_\tau &\rightharpoonup \varphi \ \text{ in } \ L^2(0,T;H^2(\Omega)), \\
\widetilde{\varphi}_\tau &\to \widetilde{\varphi} \ \text{ in } \ L^p(Q), \\
\widetilde{c}_\tau &\rightharpoonup \widetilde{c} \ \text{ in } \ L^2(0,T;H_0^1(\Omega)), \\
c_\tau &\rightharpoonup c \ \text{ in } \ L^2(0,T;H_0^1(\Omega)) \\
\widetilde{c}_\tau &\overset{*}{\rightharpoonup} \widetilde{c} \ \text{ in } \ L^\infty(0,T;L^2(\Omega)), \\
c_\tau &\overset{*}{\rightharpoonup} c \ \text{ in } \ L^\infty(0,T;L^2(\Omega)).
\end{aligned}
\tag{5.9}
$$

Since $(\widetilde{\varphi}_\tau - \varphi_\tau, \widetilde{c}_\tau - c_\tau)$ converge to 0 in $(L^2(Q))^2$, we conclude that $(\varphi, c) = (\widetilde{\varphi}, \widetilde{c})$.

We infer from (5.9) that $\varphi_\tau \to \varphi$ a.e. in Q; this and $0 \le \varphi_\tau(x,t) \le 1$ imply

$$
0 \le \varphi(x,t) \le 1 \ \text{ a.e. in Q.} \tag{5.10}
$$

Observe that from (5.9) and using the assumption **(H)**, we obtain that

$$
D_1(\varphi_\tau) \to D_1(\varphi) \ \text{ a.e. in Q.}
$$

Now, for each τ and any fixed $2 \le p < \infty$, define the functions $g_\tau = |D_1(\varphi_\tau) - D_1(\varphi)|^p$. By using again **(H)** and the previously proved almost everywhere convergences, we obtain $|g_\tau| \le 2^p \rho_1^p$ and $g_\tau \to 0$ a.e. Then, by the Lebesgue's dominated convergence theorem, we conclude that

$$
D_1(\varphi_\tau) \to D_1(\varphi) \ \text{ strongly in } \ L^p(Q), \tag{5.11}
$$

for any $2 \le p < \infty$.

Next, we need the estimate of fractional in time of $\widetilde{c}_\tau$ to apply the compactness result given in Lemma 2.4.

We set $Y = H_0^1(\Omega)$ and $X = L^2(\Omega)$; the embedding of $H_0^1(\Omega)$ in $L^2(\Omega)$ is compact by Rellich's theorem; we choose $p = 2$ and $\mathcal{G}$ is the family of functions $\widetilde{c}_\tau$.

Now, using function $(\widetilde{\varphi}_\tau, \widetilde{c}_\tau)$, and corresponding step function (φ_τ, c_τ) we rewrite **(PD)** in the form

$$
\frac{\partial \widetilde{\varphi}_\tau}{\partial t} - \xi^2 \Delta \varphi_\tau = (\varphi_\tau - 1)(1 - 2\varphi_\tau)\varphi_\tau - |\nabla \varphi_\tau| c_\tau,
$$

$$
\frac{d}{dt}\left(\int_\Omega \widetilde{c}_\tau(t)\, v\, dx \right) + \int_\Omega D_1(\varphi_\tau(t))\nabla c_\tau(t)\nabla v\, dx = \\
- \int_\Omega D_2(\varphi_\tau(t), c_\tau(t))\nabla \varphi_\tau(t) v\, dx,
\tag{5.12}
$$

for all $v \in H_0^1(\Omega)$.

We then know from Lemma 5.1 the $\widetilde{c}_\tau$ is bounded in $L^2(0,T;H_0^1(\Omega))$. There remains to show (2.6). For this, we integrate (5.12) between t and $t + a$, $t \in (0,T)$, $a > 0$:

$$
\int_\Omega (\widetilde{c}_\tau(t+a) - \widetilde{c}_\tau(t))v\, dx =
$$

$$
- \int_t^{t+a} \int_\Omega D_1(\varphi_\tau(s))\nabla c_\tau(s)\nabla v\, dx\, ds
$$

$$
- \int_t^{t+a} \int_\Omega D_2(\varphi_\tau(s), c_\tau(s))\nabla \varphi_\tau(s)\nabla v\, dx\, ds.
$$

We choose $v = \widetilde{c}_\tau(t+a) - \widetilde{c}_\tau(t)$, and integrate these relations between 0 and $T - a$. We find

$$
\int_0^{T-a} \|\widetilde{c}_\tau(t+a) - \widetilde{c}_\tau(t)\|_{2,\Omega}^2 = I_1 + I_2, \tag{5.13}
$$

where

$$
I_1 = - \int_0^{T-a} \int_t^{t-a} \int_\Omega D_1(\varphi_\tau(s))J_1\, dx\, ds\, dt,
$$

$$
I_2 = - \int_0^{T-a} \int_t^{t+a} \int_\Omega D_2(\varphi_\tau(s), c_\tau(s))J_2\, dx\, ds\, dt,
$$

with $J_1 = \nabla c_\tau(s)(\nabla \widetilde{c}_\tau(t+a) - \nabla \widetilde{c}_\tau(t))$ and $J_2 = \nabla \varphi_\tau(s)(\nabla \widetilde{c}_\tau(t+a) - \nabla \widetilde{c}_\tau(t))$.

Using the assumptions **(H)**, Fubini's theorem and Schwarz inequality, we get

$$
|I_1| \le \rho_1 T^{1/2} a^{1/2} \left(\int_0^T \|\nabla c_\tau(s)\|_{2,\Omega}^2 ds \right)^{1/2}
$$

$$
\left(\int_0^{T-a} \|\nabla \widetilde{c}_\tau(t+a) - \nabla \widetilde{c}_\tau(t)\|_{2,\Omega}^2 dt \right)^{1/2},
$$

$$
|I_2| \le \rho_2 T^{1/2} a^{1/2} \left(\int_0^T \|\nabla \varphi_\tau(s)\|_{2,\Omega}^2 ds \right)^{1/2}
$$

$$
\left(\int_0^{T-a} \|\nabla \widetilde{c}_\tau(t+a) - \nabla \widetilde{c}_\tau(t)\|_{2,\Omega}^2 dt \right)^{1/2}.
$$

From Lemma 5.1, we obtain

$$
|I_1| \le M\, a^{1/2}, \quad |I_2| \le M\, a^{1/2}. \tag{5.14}
$$

Combining (5.14) and (5.13), we obtain (2.6). Hence there exist subsequences still note c_τ, such that as $\tau \to 0$,

$$
c_\tau \to c \ \text{ in } \ L^2(Q). \tag{5.15}
$$

— 5 —

Applying arguments that are similar to the ones used to obtain the estimate (5.11), we can show the following convergence:

$$D_2(\varphi_\tau, c_\tau) \to D_2(\varphi, c) \text{ strongly in } L^p(Q),$$

with $2 \le p < \infty$.

On the other hand, for any $\psi \in L^2(Q)$, we have that

$$\int_Q ((3\varphi_\tau^2 - 2\varphi_\tau^3 - \varphi_\tau) - (3\varphi^2 - 2\varphi^3 - \varphi))\psi \, dx \, dt =$$

$$\int_Q d_\tau (\varphi_\tau - \varphi)\psi \, dx \, dt,$$

where $d_\tau = 3(\varphi_\tau + \varphi) - 2(\varphi_\tau^2 + \varphi_\tau \varphi + \varphi^2) - 1$. We observe that by using the fact that $0 \le \varphi_\tau \le 1$ and $0 \le \varphi \le 1$ we obtain $||d_\tau||_{\infty,Q} \le M$. Consequently, $\int_Q d_\tau (\varphi_\tau - \varphi)\psi \, dx \, dt \le ||d||_{\infty,Q} ||\varphi_\tau - \varphi||_{2,Q} ||\psi||_{2,Q}$, and from (5.9), we conclude that

$$\varphi_\tau(\varphi_\tau - 1)(1 - 2\varphi_\tau) \rightharpoonup \varphi(\varphi - 1)(1 - 2\varphi) \text{ in } L^2(Q).$$

Moreover, from (5.9) and (5.15), we conclude that

$$|\nabla\varphi_\tau| \, c_\tau \rightharpoonup |\nabla\varphi| \, c \text{ in } L^2(Q).$$

With the previous convergence results, with standard arguments, it is easy to take the limit in the approximate problem **(PD)** and prove that φ and c is the required solution.

This completes the proof of Theorem 2.2. ∎

6 Proof of Theorem 2.3

To examine the regularity of (φ, c), we assume that $D_1(s) \in C^1(\mathbb{R})$ and $D_2(s, y) \in C^1(\mathbb{R}^2)$ such that

$$|\partial_s D_1| \le \rho_2, \quad |\partial_s D_2| \le \alpha_1, \quad |\partial_y D_2| \le \alpha_2, \tag{6.16}$$

where $\rho_2, \alpha_1, \alpha_2 \in \mathbb{R}^+$.

Now, we multiplying the second equation in **(PD)** by $-2\tau\Delta c^m$, integrating over Ω and using Green's formula, we obtain

$$2\int_\Omega (\nabla c^m - \nabla c^{m-1})\nabla c^m \, dx +$$

$$2\tau \int_\Omega D_1(\varphi^m)|\Delta c^m|^2 \, dx =$$

$$2\tau \int_\Omega \partial_\varphi D_1(\varphi^m)\nabla\varphi^m \nabla c^m \Delta c_m \, dx -$$

$$2\tau \int_\Omega \partial_\varphi D_2(c^m, \varphi^m)|\nabla\varphi^m|^2 \Delta c^m \, dx -$$

$$2\tau \int_\Omega \partial_c D_2(c^m, \varphi^m)\nabla\varphi^m \nabla c^m \Delta c^m \, dx -$$

$$-2\tau \int_\Omega D_2(c^m, \varphi^m)\Delta\varphi^m \Delta c^m \, dx. \tag{6.17}$$

Using the assumptions **(H)** and (6.16), the estimate (2.4), Hölder's and Young's inequalities, we obtain

$$||\nabla c^m||_{2,\Omega}^2 - ||\nabla c^{m-1}||_{2,\Omega}^2 +$$
$$||\nabla c^m - \nabla c^{m-1}||_{2,\Omega}^2 + \frac{\tau\rho_0}{8}||\Delta c^m||_{2,\Omega}^2 \le$$

$$\tau M_1 ||\nabla\varphi^m||_{4,\Omega}^2 ||\nabla c^m||_{4,\Omega}^2 +$$
$$\tau M_2 ||\nabla\varphi^m||_{4,\Omega}^4 + \tau M_3 ||\Delta\varphi^m||_{2,\Omega}^2.$$

From the interpolation result (2.1) and (4.8), we obtain

$$||\nabla\varphi^m||_{4,\Omega}^2 \le M||\Delta\varphi^m||_{2,\Omega}, \tag{6.18}$$

and consequently, we have

$$||\nabla c^m||_{2,\Omega}^2 - ||\nabla c^{m-1}||_{2,\Omega}^2 +$$
$$||\nabla c^m - \nabla c^{m-1}||_{2,\Omega}^2 + \frac{\tau\rho_0}{8}||\Delta c^m||_{2,\Omega}^2 \le$$

$$\tau M_4 ||\Delta\varphi^m||_{2,\Omega}||\nabla c^m||_{2,\Omega}||\Delta c^m||_{2,\Omega} +$$
$$\tau M_5 ||\Delta\varphi^m||_{2,\Omega}^2.$$

Applying Young's inequalitly, we get

$$||\nabla c^m||_{2,\Omega}^2 - ||\nabla c^{m-1}||_{2,\Omega}^2 +$$
$$||\nabla c^m - \nabla c^{m-1}||_{2,\Omega}^2 + \frac{\tau\rho_0}{16}||\Delta c^m||_{2,\Omega}^2 \le$$

$$\tau M_6 ||\Delta\varphi^m||_{2,\Omega}^2 ||\nabla c^m||_{2,\Omega}^2 +$$
$$\tau M_5 ||\Delta\varphi^m||_{2,\Omega}^2.$$

Summing these relations for $m = 1, 2, ..., r$, with $1 \le r \le N$, we find

$$||\nabla c^r||_{2,\Omega}^2 + \sum_{m=1}^r ||\nabla c^m - \nabla c^{m-1}||_{2,\Omega}^2 +$$

$$\tau \sum_{m=1}^r ||\Delta c^m||_{2,\Omega}^2 \le M_7 \Big(||\nabla c_0||_{2,\Omega}^2 +$$

$$\tau \sum_{m=1}^N ||\Delta\varphi^m||_{2,\Omega}^2 ||\nabla c^m||_{2,\Omega}^2 + \tau \sum_{m=1}^N ||\Delta\varphi^m||_{2,\Omega}^2 \Big).$$

From Lemma 5.1 and discrete Gronwall Lemma 2.3, we obtain

$$\max_{1 \le r \le N} ||\nabla c^r||_{2,\Omega} + \tau \sum_{m=1}^r ||\Delta c^m||_{2,\Omega}^2 +$$

$$\sum_{m=1}^r ||\nabla c^m - \nabla c^{m-1}||_{2,\Omega}^2 \le$$

$$M_8\Big(1 + ||\varphi_0||^2_{H^1(\Omega)} + ||c_0||^2_{H^1(\Omega)}\Big). \quad (6.19)$$

Now, we multiplying the concentration equation in **(PD)** by $\delta_t c^m$, integrating over Ω and using Green's formula, we obtain

$$||\delta_t c^m||^2_{2,\Omega} = \int_\Omega \partial_\varphi D_1(\varphi^m)\nabla\varphi^m\nabla c^m \delta_t c^m \, dx +$$

$$\int_\Omega D_1(\varphi^m)\Delta c^m \delta_t c^m \, dx -$$

$$\int_\Omega \partial_\varphi D_2(c^m,\varphi^m)|\nabla\varphi^m|^2 \delta_t c^m \, dx -$$

$$\int_\Omega \partial_c D_2(c^m,\varphi^m)\nabla\varphi^m\nabla c^m \delta_t c^m \, dx -$$

$$\int_\Omega D_2(c^m,\varphi^m)\Delta\varphi^m \delta_t c^m \, dx.$$

Using the assumptions **(H)** and (6.16), Hölder's and Young's inequalities, we obtain

$$||\delta_t c^m||^2_{2,\Omega} \leq M_9\Big(||\nabla\varphi^m||^2_{4,\Omega}||\nabla c^m||^2_{4,\Omega} +$$

$$||\nabla\varphi^m||^4_{4,\Omega} + ||\Delta\varphi^m||^2_{2,\Omega} + ||\Delta c^m||^2_{2,\Omega}\Big).$$

From (2.3) and (6.18), we get

$$||\delta_t c^m||^2_{2,\Omega} \leq$$

$$M_{10}\Big(||\Delta\varphi^m||_{2,\Omega}||\nabla c^m||_{2,\Omega}||\Delta c^m||_{2,\Omega} +$$

$$||\Delta\varphi^m||^2_{2,\Omega} + ||\Delta c^m||^2_{2,\Omega}\Big).$$

Applying Young's inequality, we have

$$\tau||\delta_t c^m||^2_{2,\Omega} \leq$$

$$\tau M_{11}\Big(||\Delta\varphi^m||^2_{2,\Omega}||\nabla c^m||^2_{2,\Omega} +$$

$$||\Delta\varphi^m||^2_{2,\Omega} + ||\Delta c^m||^2_{2,\Omega}\Big).$$

Summing these relations for $m = 1, 2, ..., N$, we find

$$\tau\sum_{m=1}^N ||\delta_t c^m||^2_{2,\Omega} \leq M_{11}\left(\max_{1\leq m\leq N}||\nabla c^m||^2_{2,\Omega}\right.$$

$$\left(\tau\sum_{m=1}^N ||\Delta\varphi^m||^2_{2,\Omega}\right) +$$

$$\left.\tau\sum_{m=1}^N ||\Delta\varphi^m||^2_{2,\Omega} + \tau\sum_{m=1}^N ||\Delta c^m||^2_{2,\Omega}\right).$$

From Lemma 5.1 and (6.19), we obtain

$$\tau\sum_{m=1}^N ||\delta_t c^m||^2_{2,\Omega} \leq M_{12}\Big(||\varphi_0||^2_{H^1(\Omega)} + ||c_0||^2_{H^1(\Omega)}\Big),$$

where the constant M_{12} depends on T, ξ^2, ξ^4, ρ_l, α_l, $|\Omega|$, $||\varphi_0||_{2,\Omega}$ and $||c_0||_{2,\Omega}$ with $l = 1, 2$.

This completes the proof of Theorem 2.3. ∎

References

[1] C. Beckermann, H.J. Diepers, I. Steinbach, A. Karma and X. Tong, *Modeling melt convection in phase-field simulations of solidification*, J. Comp. Phys.,154, 468, 1999.

[2] G. Caginalp and W. Xie, *Phase-Field and sharp-interface alloy models*, Arch. Rat. Mech. Anal., 92, 205, 1986.

[3] K. Deimling, *Nonlinear Functional Analysis*, Springer-Verlag, 1984.

[4] H.J. Diepers, C. Berckermann and C. Steinbach, *Simulation of convection and repenting a binary alloy mush using the Phase-field method*, Acta. Mater., vol 47,13, 3663, 1999.

[5] L. C. Evans, *Partial Differential Equations*, American Mathematical Society, vol 19, 1998.

[6] D. Henry, *Geometric Theory of Semilinear Parabolic Equations*, Lecture Notes in Mathematics 840, Springer-Verlag, Berlin Heildelberg, 1981.

[7] K.H. Hoffman and L. Jiang, *Optimal Control a phase field model for solidification*, Numer. Funct. Anal. Optimiz. 13 (1 & 2), 11, 1992.

[8] O.A. Ladyzenskaja, V.A. Solonnikov, N.N. Ural'ceva, *Linear and Quasilinear Equations of Parabolic Type*, American Mathematical Society, Providence, 1968.

[9] J.L. Lions, *Control of distributed singular systems*. Gauthier-Villars, 1985.

[10] C. Moroşanu and D. Motreanu, *A generalized phase-field system*, J. Math. Anal. Appl., vol. 273, 1999, 515-540.

[11] J. Rappaz and J.F. Sheid, *Existence of solutions to a phase-field model for the isothermal solidification process of binary alloy*, Math. Methods Appl. Sci., 23(6)(2000), 491-513.

[12] R. Temam, Navier-Stokes Equations, Theory and Numerical Analysis, North-Holland Publishing Company, 1977.

[13] S. Zheng *Nonlinear parabolic equations and hyperbolic-parabolic coupled system*, Pitman Monographs and Surveys in Pure and Applied Mathematics, 76, Longman, 1995.