ON CAHN-HILLIARD SYSTEMS WITH ELASTICITY

HARALD GARCKE

ABSTRACT. Elastic effects can have a pronounced effect on the phase separation process in solids. The classical Ginzburg-Landau energy can be modified to account for such elastic interactions. The evolution of the system is then governed by diffusion equations for the concentrations of the alloy components and by a quasi-static equilibrium for the mechanical part. The resulting system of equations is elliptic-parabolic and can be understood as a generalisation of the Cahn-Hilliard equation. In this paper we give a derivation of the system and prove an existence and uniqueness result for it.

1. INTRODUCTION

We study a mathematical model describing phase separation in multicomponent alloys in the presence of elastic interactions. Our aim is to describe the following phenomena. At temperatures larger than a critical temperature θ_c, one homogeneous phase characterised by a certain mixture of the alloy components is energetically favourable. If the temperature is decreased below θ_c two or more phases develop and the system rapidly decomposes into a microstructure consisting of many regions with different phases. Each phase is characterised by a distinct composition of the individual components and these are such that the bulk chemical energy becomes small. The formation of the microstructure is on a very fast time scale and is called spinodal decomposition or phase separation. One observes the development of many connected regions of distinct phases which we call particles.

Associated with the interfaces between phases is an interfacial energy. Since the phases are finely mixed, the interfacial energy is large after spinodal decomposition. In a second stage of the evolution, the

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microstructure coarsens and hence the interfacial energy decreases. In the case of negligible elastic effects, particles tend to become round, small particles shrink and larger ones grow. This part of the evolution called coarsening (or Ostwald ripening) is mainly driven by the reduction of the total amount of interfacial area.

If the components of the mixture have different elastic moduli or different lattice structure, elastic effects might influence the rate of coarsening and the morphology of the particles. Elastic effects can result for example from different lattice spacing's of the alloy components. We refer to Garcke, Rumpf, Weikard [25] for numerical simulations that demonstrate the effects that anisotropic elastic energy and different lattice spacing's can have on the coarsening morphology. The elastic effects become more important at later stages of the evolution. This can be seen by comparing the energy of the elastic and surface energy (see Fratzl, Penrose, Lebowitz [20]). Furthermore numerical simulations indicate this (see [25]).

In applications of multi-component alloys it is important to know the rate of coarsening. The famous theory of Lifshitz, Slyozov [34] and Wagner [45] (LSW-theory) says that the average particle size in systems driven by diffusion without stress effects is proportional to $t^{\frac{1}{3}}$. If stress effects cannot be neglected then an approach like in the LSW-theory does not seem to be possible and the late stage evolution in phase separating systems with elastic effects is not yet very well understood.

Material scientists hoped to find situations in which stress effects can slow down the rate of coarsening. Some experiments even suggested that inverse coarsening is possible, i.e. the average domain size decreases (see e.g. [19, 20, 28, 31, 36, 35, 37, 38]). The understanding of the mechanisms responsible for these effects is very important for technological applications. A uniform distribution of regions of different phases is desirable in order to guarantee evenly distributed material properties of the sample. For example mechanical properties such as the strength and the mechanical stability of the material depend on how finely mixed regions of different phases are. The control of aging and therefore of the lifetime of materials depends on the ability to understand the coarsening process. This demonstrates the importance of a reliable mathematical model to describe phase separation in multi-component solids in the presence of elastic interactions.

In Section 2 we introduce a model for phase transformations in solids taking elastic effects into account. The free energy of the system is a Ginzburg-Landau functional defined in terms of the concentrations of the individual components and the displacement of the lattice. Interfaces are described by a transition layer of finite but small thickness. Two terms in the Ginzburg-Landau free energy are classical. The first one is quadratic in the gradients of the concentrations and penalises large gradients. The other represents the bulk chemical energy and in the case of phase separation its density is a non-convex function of the concentrations. In order to model effects due to stresses we also include elastic terms in the Ginzburg-Landau free energy. Since in the phenomena we are interested in, the strain is typically small, we present a geometrically linear theory formulated in terms of the linearised strain tensor.

The evolution of the system is governed by diffusion equations for the concentrations of the individual components and a quasi-static equilibrium for the mechanical part. The latter condition is reasonable since the mechanical equilibrium is obtained on a much faster time scale than diffusion takes place. The overall system consists of a system of fourth order parabolic diffusion equations coupled to an elliptic system describing mechanical equilibrium. In the two component case with no elastic interactions the elliptic-parabolic system reduces to the standard scalar Cahn-Hilliard equation.

In the third section we prove an existence result for the elliptic-parabolic system. In order to obtain approximate solutions of the problem we use the method of implicit time discretisation and at each time step solve a minimum problem taking into account the variational structure. A major difficulty of the analysis is the fact that the displacement gradient enters the diffusion equation quadratically. Hence, it is necessary to show strong convergence of the displacement gradient in L^2. We also state a uniqueness result (Section 4) in the case of linear elasticity under the assumption of homogeneous elasticity, i.e. the elasticity tensor is independent of the concentrations. In an appendix we collect some results used in this work and finally we list our notation.

Let us mention other papers on the Cahn-Hilliard equation related to this work (for an overview on the Cahn-Hilliard equation see Elliott [11] and Novick-Cohen [39]). Existence results for the scalar Cahn-Hilliard equation without elasticity have been given by Elliott and Zheng Songmu [15] for the case of a smooth free energy density, by Elliott and Luckhaus [14] for the case of a logarithmic free energy density and by Blowey and Elliott [5] for the case of a free energy density of obstacle type. The results of Elliott and Luckhaus [14] also hold for systems. For more results on Cahn-Hilliard systems we refer to Eyre [18], Bronsard, Garcke and Stoth [7] and Garcke and Novick-Cohen [24].

We already refered to the work by material scientists on the Cahn-Hilliard equation taking elasticity into account. The first mathematical results on this problem are due to Carrive, Miranville and Piétrus [9] and Garcke [21]. Carrive, Miranville and Piétrus [9] proved an existence result in the scalar case with homogeneous elasticity. This especially implies that the elasticity terms enter the diffusion equation equation only linearly. In this paper instead we deal with the more difficult case of heterogeneous elasticity which in particular implies that the strain enters the diffusion equation in a nonlinear way. Several variations and extensions of the model have been studied recently (see e.g. [6, 22]). We refer to Bonetti et al. [6] for the study of a viscous Cahn-Hilliard equation with elasticity and to Garcke [22] for the analysis of a model with a logarithmic free energy density.

Other descriptions of phase separation in alloys use models based on a sharp interface description of phase boundaries. In Leo, Lowengrub and Jou [33] the sharp interface limit of a Cahn-Hilliard equation with elasticity is identified with the help of formally matched asymptotic expansions. Garcke [23] identifies the Γ-limit of the free energy in the sharp interface limit in the presence of elastic interactions.

There have been several numerical studies for the Cahn-Hilliard equation with elasticity. Most of them are based on Fourier transforms and spectral methods (see Dreyer and Müller [10], Leo, Lowengrub and Jou [33] and the references therein). For numerical studies with a finite element method and a numerical analysis of this approach we refer to Garcke, Rumpf and Weikard [25].

2. The Cahn-Hilliard model with elasticity

Assume the alloy consists of N components. We denote by c_k ($k = 1, ..., N$) the concentration of component k and therefore, the vector $\mathbf{c} = (c_k)_{k=1,...,N}$ has to fulfil the constraint $\sum_{k=1}^N c_k = 1$, i.e. $\mathbf{c}$ lies in the affine hyperplane

$$\Sigma := \{\mathbf{c}' = (c'_k)_{k=1,...N} \in \mathrm{I\!R}^N \mid \sum_{k=1}^{N} c'_k = 1\,\}.$$

To describe elastic effects we define the displacement field $\mathbf{u}(\mathbf{x})$, i.e. a material point $\mathbf{x}$ in the undeformed body will be at the point $\mathbf{x} + \mathbf{u}(\mathbf{x})$

after deformation. Since in phase separation processes the displacement gradient usually is small, we consider an approximative theory based on the linearised strain tensor

$$\mathcal{E}(\mathbf{u}) = \tfrac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^t\right).$$

A generalised Ginzburg-Landau free energy taking elastic effects into account is of the form

$$E(\mathbf{c},\mathbf{u}) = \int_\Omega \left\{\tfrac{1}{2}\nabla\mathbf{c} : \mathbf{\Gamma}\nabla\mathbf{c} + \Psi(\mathbf{c}) + W(\mathbf{c},\mathcal{E}) + W^*(\mathcal{E})\right\} \tag{2.1}$$

where $\Omega \subset \mathrm{I\!R}^n$, $n \in \mathrm{I\!N}$, is a bounded domain with Lipschitz boundary and $:$ is the euclidian inner product of two tensors. The first term in the energy is the gradient part penalising rapid spatial variations in the concentrations. The tensor $\mathbf{\Gamma}$ mapping $\mathrm{I\!R}^{N\times n}$ into itself is assumed to be symmetric and positive definite. The second summand Ψ is the homogeneous (or "coarse grain") free energy density at zero stress taking into account the chemical energy of the system. The function Ψ depends on temperature and is convex above a critical temperature θ_c and non-convex for temperatures less than the critical temperature. In the latter case Ψ has several local minimisers giving rise to the appearance of different phases. These first summands in the total free energy E are classical contributions to a Ginzburg-Landau free energy. Energies consisting of two terms of this form go back to van der Waal's [44]. In the theory of phase separation in alloys they have been introduced by Cahn and Hilliard [8].

The last two terms in the free energy take elastic effects into account. The term $W(\mathbf{c},\mathcal{E})$ is the elastic free energy density and a typical form is

$$W(\mathbf{c},\mathcal{E}) = \tfrac{1}{2}\left(\mathcal{E} - \mathcal{E}^\star(\mathbf{c})\right) : \mathcal{C}(\mathbf{c})\left(\mathcal{E} - \mathcal{E}^\star(\mathbf{c})\right). \tag{2.2}$$

Here, $\mathcal{C}(\mathbf{c})$ is the concentration dependent elasticity tensor mapping symmetric tensors in $\mathrm{I\!R}^{n\times n}$ into itself. We require $\mathcal{C}(\mathbf{c})$ to be symmetric and positive definite. The quantity $\mathcal{E}^\star(\mathbf{c})$ is the symmetric stress free strain (or eigenstrain) at concentration $\mathbf{c}$. This is the value the strain tensor attains if the material were uniform with concentration $\mathbf{c}$ and unstressed. If the vector $\mathbf{c}$ is equal to one of the standard cartesian basis vectors $\mathbf{e}_1, ..., \mathbf{e}_N$ then the system is equal to a pure component. Hence, $\mathcal{E}^\star(\mathbf{e}_k)$ is the value of the strain tensor if the material consists only of component k and is unstressed. The function $\mathcal{E}^\star$ is a suitable extension to all of Σ. Usually a linear extension of the form

$$\mathcal{E}^\star(\mathbf{c}) = \sum_{k=1}^N c_k \mathcal{E}^\star(\mathbf{e}_k)$$

is assumed (Vegard's law). The elastic energy density (2.2) is the standard choice which goes back to the early work of Eshelby [16] and Khachaturyan [29] (see also [33, 20]). However, we will obtain results for more general densities.

The remaining term $W^\star(\mathcal{E})$ represents energy effects due to externally applied forces. For simplicity, we assume that there are no body forces and that the boundary tractions are dead loads given by a constant and symmetric tensor $\mathcal{S}^*$, i.e. the tractions applied to $\partial\Omega$ are given by $\mathcal{S}^*\mathbf{n}$. The work needed to bring the undeformed body into the state with displacement $\mathbf{u} : \Omega \to \mathbb{R}^3$ is then given by

$$-\int_{\partial\Omega} \mathbf{u} \cdot \mathcal{S}^*\mathbf{n} = -\int_\Omega \nabla\mathbf{u} : \mathcal{S}^* = -\int_\Omega \mathcal{E}(\mathbf{u}) : \mathcal{S}^*,$$

where $\mathbf{n}$ is the outer unit normal to Ω. Hence,

$$W^*(\mathcal{E}') := -\mathcal{E}' : \mathcal{S}^*$$

is the energy density of the applied outer forces.

To describe evolution phenomena in the system, we consider mass diffusion for the individual components leading to diffusion equations for the concentrations. Mechanical equilibrium is attained on a much faster time scale than diffusion takes place. Therefore, we will assume a quasi-static equilibrium for $\mathbf{u}$, i.e. for all times

$$\nabla \cdot \mathcal{S} = 0,$$

where

$$\mathcal{S} = W_{,\mathcal{E}}(\mathbf{c}, \mathcal{E}(\mathbf{u}))$$

is the stress tensor. We remark that the solution of the elastic system in general depends on time since $\mathbf{c}$ in general is time dependent. It is always assumed that W depends on its second argument only through its symmetric part, i.e. $W(\mathbf{c}', \mathcal{E}') = W(\mathbf{c}', (\mathcal{E}')^t)$. This implies that $\mathcal{S} = W_{,\mathcal{E}}(\mathbf{c}', \mathcal{E}')$ is symmetric.

The diffusion equations for the concentrations c_k $(k = 1, ..., N)$ are based on mass balances for the individual components. To define the mass balance we need to introduce chemical potentials μ_k which are defined as the variational derivative of the total free energy E with respect to c_k, i.e.

$$\mu_k = -(\nabla \cdot \mathbf{\Gamma}\nabla\mathbf{c})_k + \Psi_{,c_k}(\mathbf{c}) + W_{,c_k}(\mathbf{c}, \mathbf{u}).$$

Now Onsager's postulate [40, 41, 30] says that each thermodynamic flux is linearly related to every thermodynamic force. Since in our case the thermodynamic forces are the negative chemical potential gradients, we obtain the phenomenological equations (see Kirkaldy and Young [30], p. 137)

$$\mathbf{J}_k = -\sum_{l=1}^{N} L_{kl} \nabla \mu_l \tag{2.3}$$

with a constant matrix $\mathbf{L} = (L_{kl})_{k=1,\ldots,N;l=1,\ldots,N} \in \mathrm{I\!R}^{N\times N}$. The Onsager reciprocity law (see [30], p. 137, and [40, 41]) states that the matrix $\mathbf{L}$ has to be symmetric, which we assume in the following. Having defined the flux, the diffusion equations follow from the balance of mass as

$$\partial_t c_k = -\nabla \cdot \mathbf{J}_k. \tag{2.4}$$

To ensure that the diffusion equations (2.4) are consistent with the constraint $\sum_{k=1}^{N} c_k = 1$ the fluxes have to fulfil a linear dependency of the form

$$\sum_{k=1}^{N} \mathbf{J}_k = 0. \tag{2.5}$$

Since the identities (2.3) and (2.5) have to hold for all possible chemical potentials we have to impose

$$\sum_{l=1}^{N} L_{kl} = 0. \tag{2.6}$$

This property of the mobility matrix $\mathbf{L} = (L_{kl})_{k=1,\ldots,N;l=1,\ldots,N}$ we assume from now on. As a consequence the diffusion equations (2.4) become

$$\begin{aligned} \partial_t c_k &= \nabla \cdot \left(\sum_{l=1}^{N} L_{kl} \nabla \mu_l \right) \\ &= \sum_{l=1}^{N} L_{kl} \Delta \tfrac{1}{N} \sum_{m=1}^{N} (\mu_l - \mu_m). \end{aligned}$$

Hence, the diffusion equations can be expressed via the chemical potential differences $(\mu_l - \mu_k)$. In particular, the evolution can be described via the vector of generalised chemical potential differences

$$\begin{aligned} \mathbf{w} &= \tfrac{1}{N} \left(\sum_{m=1}^{N} (\mu_l - \mu_m) \right)_{l=1,\ldots,N} \\ &= \mathbf{P}\boldsymbol{\mu} \end{aligned}$$

where $\mathbf{P}$ is the euclidian projection of $\mathrm{I\!R}^N$ onto

$$T\Sigma = \{ \mathbf{d}' = (d'_k)_{k=1,\ldots N} \in \mathrm{I\!R}^N \mid \sum_{k=1}^{N} d'_k = 0 \}$$

which is the tangent space to Σ. A simple computation yields that $\mathbf{w}$ is the variational derivative of E when one takes the constraint $\sum_{k=1}^{N} c_k = 1$ into account. In fact, introducing $\mathbf{e} = (1, ..., 1)$, we get $\mathbf{w} = \boldsymbol{\mu} - \frac{1}{N}(\boldsymbol{\mu} \cdot \mathbf{e})\mathbf{e}$ where the second term is the Lagrange multiplier associated to the constraint $\sum_{k=1}^{N} c_k = 1$.

Altogether we obtain the system of equations

$$\begin{aligned} \partial_t \mathbf{c} &= \mathbf{L}\Delta \mathbf{w}, && (2.7)\\ \mathbf{w} &= \mathbf{P}\left(-\nabla \cdot \boldsymbol{\Gamma}\nabla \mathbf{c} + \Psi_{,\mathbf{c}}(\mathbf{c}) + W_{,\mathbf{c}}(\mathbf{c}, \mathcal{E}(\mathbf{u}))\right), && (2.8)\\ \nabla \cdot \mathcal{S} &= 0, && (2.9)\\ \mathcal{S} &= W_{,\mathcal{E}}(\mathbf{c}, \mathcal{E}(\mathbf{u})). && (2.10) \end{aligned}$$

If only two components are present, one can use the constraint $c_1 + c_2 = 1$ to reduce the system for the concentrations to a single equation. In this case the equations (2.7)-(2.10) were first stated by Larché and Cahn [32] for $\gamma = 0$ and for nonzero γ by Onuki [42].

As boundary conditions we impose no-flux conditions for the $\mathbf{J}_k$ and the natural boundary conditions which one obtains from variations of the energy functional with respect to $\mathbf{c}$ and $\mathbf{u}$. Therefore, with $\mathbf{n}$ being the outer unit normal to Ω, we require

$$\begin{aligned} \mathbf{L}\nabla \mathbf{w} \cdot \mathbf{n} &= 0, && (2.11)\\ \boldsymbol{\Gamma}\nabla \mathbf{c} \cdot \mathbf{n} &= 0, && (2.12)\\ \mathcal{S} \cdot \mathbf{n} &= \mathcal{S}^* \cdot \mathbf{n}. && (2.13) \end{aligned}$$

In addition, we impose initial conditions for $\mathbf{c}$, i.e.

$$\mathbf{c}(\mathbf{x}, 0) = \mathbf{c}^0(\mathbf{x}) \qquad (2.14)$$

for a given function $\mathbf{c}^0$ with $\mathbf{c}^0(\mathbf{x}) \in \Sigma$ for all $\mathbf{x} \in \Omega$. Since we assume that the mechanical equilibrium is obtained instantaneously no initial conditions for $\mathbf{u}$ are needed. We remark that the no-flux boundary condition implies that the total mass of the solution to (2.7)-(2.14) is a conserved quantity, i.e. for all times $t > 0$

$$\int_\Omega \mathbf{c}(\mathbf{x}, t)d\mathbf{x} = \int_\Omega \mathbf{c}^0(\mathbf{x})d\mathbf{x}.$$

Other boundary conditions are possible. For example we could impose Dirichlet conditions for $\mathbf{u}$ on parts of the boundary $\partial\Omega$. This means to prescribe the deformation on parts of the boundary and hence a unique $\mathbf{u}$ could be determined. The boundary condition (2.13) on the other hand prescribes $\mathbf{u}$ only up to infinitesimal rigid displacements (i.e. translations and infinitesimal rotations). This is typical for problems in elasticity that are based on a linearised strain tensor $\mathcal{E}$. The non-uniqueness in $\mathbf{u}$ will have no effect on the evolution of $\mathbf{c}$ since only $\mathcal{E}(\mathbf{u})$ enters the equation for $\mathbf{w}$.

The above system of equations is thermodynamically consistent if the second law of thermodynamics holds. For isothermal systems the second law is equivalent to a dissipation inequality for the free energy. Using the equations (2.7)-(2.10) and the symmetry of $\mathcal{S}$ and $\mathcal{S}^*$ we compute formally:

$$
\begin{aligned}
&\partial_t\big(\tfrac{1}{2}\nabla\mathbf{c} : \mathbf{\Gamma}\nabla\mathbf{c} + \Psi(\mathbf{c}) + W(\mathbf{c},\mathcal{E}) + W^*(\mathcal{E})\big) = \\
&\quad = \mathbf{\Gamma}\nabla\mathbf{c} : \nabla\partial_t\mathbf{c} + \Psi_{,\mathbf{c}}\cdot\partial_t\mathbf{c} + W_{,\mathbf{c}}\cdot\partial_t\mathbf{c} + W_{,\mathcal{E}} : \partial_t\mathcal{E} - \mathcal{S}^* : \partial_t\mathcal{E} \\
&\quad = \nabla\cdot\{\mathbf{\Gamma}\nabla\mathbf{c}\cdot\partial_t\mathbf{c} + \mathcal{S}\partial_t\mathbf{u} - \mathcal{S}^*\partial_t\mathbf{u}\} + \{-\nabla\cdot\mathbf{\Gamma}\nabla\mathbf{c} + \Psi_{,\mathbf{c}} + W_{,\mathbf{c}}\}\cdot\partial_t\mathbf{c} \\
&\quad = \nabla\cdot\{\mathbf{\Gamma}\nabla\mathbf{c}\cdot\partial_t\mathbf{c} + \mathcal{S}\partial_t\mathbf{u} - \mathcal{S}^*\partial_t\mathbf{u} - \mathbf{J}\cdot\boldsymbol{\mu}\} - \nabla\boldsymbol{\mu} : \mathbf{L}\nabla\boldsymbol{\mu}.
\end{aligned}
$$

Hence, assuming that $\mathbf{L}$ is positive semidefinite, we obtain the local dissipation inequality

$$
\begin{aligned}
&\partial_t\Big(\tfrac{1}{2}\nabla\mathbf{c} : \mathbf{\Gamma}\nabla\mathbf{c} \; + \Psi(\mathbf{c}) + W(\mathcal{E},\mathbf{c}) + W^*(\mathcal{E})\Big) \leq \\
&\qquad\qquad \leq \nabla\cdot\{\mathbf{\Gamma}\nabla\mathbf{c}\cdot\partial_t\mathbf{c} + \mathcal{S}\partial_t\mathbf{u} - \mathcal{S}^*\partial_t\mathbf{u} - \mathbf{J}\cdot\boldsymbol{\mu}\}\,.
\end{aligned}
\tag{2.15}
$$

This shows that the rate of change of energy cannot exceed the total power expended plus the energy inflow. In inequality (2.15) the term $\mathcal{S}\partial_t\mathbf{u}-\mathcal{S}^*\partial_t\mathbf{u}$ denotes the power expended by deformation stresses, $\mathbf{J}\cdot\boldsymbol{\mu}$ accounts for the energy inflow by diffusion and $\mathbf{\Gamma}\nabla\mathbf{c}\cdot\partial_t\mathbf{c}$ can be interpreted to result from flow of energy due to moving phase interfaces (see [4, 26, 27]). Integrating the dissipation inequality (2.15) and using the boundary conditions shows that the free energy serves as a Lyapunov functional. In the following section the Lyapunov property of the free energy will give the main a priori estimate in the existence theory.

3. Existence for the diffuse interface system

In this section we prove an existence result for the elliptic-parabolic system. We use the fact that the system aims to decrease the free energy. In the concentration variables the system has a gradient flow structure with respect to a weighted $\big(H^1(\Omega,\mathbb{R}^N)\big)^*$-scalar product and for the mechanical part the relaxation is infinitely fast and equilibrium is achieved instantaneously. Using this property of the system we make an implicit time discretisation which leads to a variational problem in each time step. To formulate the variational problem we need to understand in which sense the system can be understood as the steepest descent of the free energy. Therefore, we introduce a suitably weighted scalar product in the dual of H^1.

3.1. **The gradient flow structure.** Let

$$X_1 := \{\mathbf{c} \in H^1(\Omega, \mathbb{R}^N) \,|\, \mathbf{c} \in \Sigma \text{ almost everywhere } \}$$

be the space of all H^1-functions fulfilling the constraint for the concentrations. Since the system (2.7)-(2.13) preserves the mean value of the vector $\mathbf{c}$, it will also be useful to introduce the spaces

$$X_1^{\mathbf{m}} := \{\mathbf{c} \in X_1 \,|\, \fint_\Omega c_k = m_k \}$$

where $\mathbf{m} = (m_k)_{k=1,...,N}$ is a constant vector of mean values with $\frac{1}{N}\sum_{k=1}^N m_k = 1$. We define the tangent space

$$Y = \{\mathbf{z} \in H^1(\Omega, \mathbb{R}^N) \,|\, \int_\Omega \mathbf{z} = 0,\ \sum_{k=1}^N z_k = 0 \}$$

of $X_1^{\mathbf{m}}$ and the space of linear functionals $\mathcal{D}$ on $H^1(\Omega, \mathbb{R}^N)$ that vanish on the L^2-complement of Y

$$\begin{aligned}\mathcal{D} \;=\; & \{\mathbf{f} \in \left(H^1(\Omega, \mathbb{R}^N)\right)^* \,|\, \langle \mathbf{d}, \mathbf{f}\rangle_{H^1,(H^1)^*} = 0 \text{ for all } \mathbf{d} = d(\mathbf{x})(1, ..., 1)\\ & \text{where } d \text{ is a scalar valued function with } d \in H^1(\Omega)\\ & \text{and for all } \mathbf{d} \equiv \mathbf{e}_k,\ k = 1, ..., N \}.\end{aligned}$$

With $\langle \mathbf{d}, \mathbf{f}\rangle$ we denote the pairing of an element $\mathbf{d}$ of a Banach space and an element $\mathbf{f}$ lying in the dual of the Banach space. Then we introduce the mapping $\mathcal{L}$ associated to the differential operator $\mathbf{z} \mapsto -\mathbf{L}\Delta\mathbf{z}$ as a mapping from Y to $\mathcal{D}$ via

$$\mathcal{L}(\mathbf{z})(\boldsymbol{\zeta}) = \int_\Omega \mathbf{L}\nabla\mathbf{z} : \nabla\boldsymbol{\zeta}.$$

The fact that $\mathcal{L}(\mathbf{z}) \in \mathcal{D}$ follows from (2.6) and the definition of Y. Later we need the inverse of the mapping $\mathcal{L}$ which we denote by $\mathcal{G}$. The invertibility of $\mathcal{L}$ follows from the Poincaré inequality and the Lax-Milgram theorem provided that $\mathbf{L}$ is positive definite on $T\Sigma$. It holds

$$(\mathbf{L}\nabla\mathcal{G}\mathbf{f}, \nabla\boldsymbol{\zeta})_{L^2} = \langle \boldsymbol{\zeta}, \mathbf{f}\rangle$$

for all $\boldsymbol{\zeta} \in H^1(\Omega, \mathbb{R}^N)$ and $\mathbf{f} \in \mathcal{D}$.

For all $\mathbf{f}_1, \mathbf{f}_2 \in \mathcal{D}$ we define the scalar product

$$(\mathbf{f}_1, \mathbf{f}_2)_{\mathbf{L}} := (\mathbf{L}\nabla\mathcal{G}\mathbf{f}_1, \nabla\mathcal{G}\mathbf{f}_2)_{L^2}$$

and the corresponding norm

$$\|\mathbf{f}\|_{\mathbf{L}} = \sqrt{(\mathbf{f}, \mathbf{f})_{\mathbf{L}}} \quad \text{for all} \quad \mathbf{f} \in \mathcal{D}.$$

Since all functions $\bar{\mathbf{f}} \in Y$ can be interpreted as elements in $\mathcal{D}$ via the mapping $\boldsymbol{\zeta} \mapsto \int_\Omega \bar{\mathbf{f}} \cdot \boldsymbol{\zeta}$ for $\boldsymbol{\zeta} \in H^1(\Omega, \mathrm{IR}^N)$ the scalar product $(.,.)_{\mathbf{L}}$ and the norm $\|.\|_{\mathbf{L}}$ are also defined for functions in Y. Using Young's inequality we obtain that for all $\delta > 0$ and all $\mathbf{d} \in Y$

$$\begin{aligned} \|\mathbf{d}\|^2_{L^2} &= (\mathbf{L}\nabla\mathcal{G}\mathbf{d}, \nabla\mathbf{d})_{L^2} \\ &\leq \|\mathbf{L}^{\frac{1}{2}}\nabla\mathcal{G}\mathbf{d}\|_{L^2}\|\mathbf{L}^{\frac{1}{2}}\nabla\mathbf{d}\|_{L^2} \\ &\leq \tfrac{C_{\mathbf{L}}}{\delta}\|\mathbf{d}\|^2_{\mathbf{L}} + \delta\|\nabla\mathbf{d}\|^2_{L^2}, \end{aligned} \tag{3.1}$$

where $C_{\mathbf{L}}$ is a constant depending on $\mathbf{L}$.

Introducing the Lagrange multiplier $\boldsymbol{\lambda}(t) = \left(⨍_\Omega \mathbf{w}\right)(t)$ we can rewrite the equation (2.7) as

$$\mathcal{G}\partial_t\mathbf{c} = \boldsymbol{\lambda} - \mathbf{w}.$$

Then the equations (2.7), (2.8) lead to

$$\begin{aligned} (\boldsymbol{\Gamma}\nabla\mathbf{c}, \nabla\boldsymbol{\zeta})_{L^2} + (\Psi_{,\mathbf{c}}(\mathbf{c}), \boldsymbol{\zeta})_{L^2} + (W_{,\mathbf{c}}(\mathbf{c}, \mathcal{E}(\mathbf{u})), \boldsymbol{\zeta})_{L^2} &= \\ &= (\mathbf{w}, \boldsymbol{\zeta})_{L^2} \\ &= -\,(\mathcal{G}\partial_t\mathbf{c}, \boldsymbol{\zeta})_{L^2} \\ &= -\,(\mathbf{L}\nabla\mathcal{G}\partial_t\mathbf{c}, \nabla\mathcal{G}\boldsymbol{\zeta})_{L^2} \\ &= -\,(\partial_t\mathbf{c}, \boldsymbol{\zeta})_{\mathbf{L}} \end{aligned}$$

which holds for all $\boldsymbol{\zeta} \in Y$. The left hand side in the above computation is the differential $D_{\mathbf{c}}E(\mathbf{c}, \mathbf{u})$ in the direction $\boldsymbol{\zeta}$. Consequently,

$$\langle\boldsymbol{\zeta}, D_{\mathbf{c}}E(\mathbf{c}, \mathbf{u})\rangle = -\,(\boldsymbol{\zeta}, \partial_t\mathbf{c})_{\mathbf{L}} \text{ for all } \boldsymbol{\zeta} \in Y, \tag{3.2}$$

which means that (2.7), (2.8) can be interpreted as the steepest descent of E in $X_1^{\mathbf{m}}$ with respect to the $(.,.)_{\mathbf{L}}$ scalar product and the variable $\mathbf{c}$. The fact that the evolution for $\mathbf{c}$ has this gradient flow structure will be used in the implicit time discretisation.

Since we consider boundary conditions of the second type, it will turn out that for fixed concentrations $\mathbf{c}$ the displacement $\mathbf{u}$ is only determined up to translations and infinitesimal rotations, i.e. up to infinitesimal rigid displacements. We note that the strain $\mathcal{E}$ is uniquely determined and hence in the evolution equation for $\mathbf{c}$ the non-uniqueness of $\mathbf{u}$ will not play any role. This discussion motivates the introduction of the space

$$X_2 := \{\mathbf{u} \in H^1(\Omega, \mathrm{IR}^n) \,|\, (\mathbf{u}, \mathbf{v})_{H^1} = 0 \text{ for all } \mathbf{v} \in X_{ird}\} = X_{ird}^{\perp},$$

where

$$\begin{aligned} X_{ird} \;:=\; \{\mathbf{u} \in H^1(\Omega, \mathrm{IR}^n) \,|\, & \text{ there exist } \mathbf{b} \in \mathrm{IR}^n \text{ and a skew symmetric} \\ & \mathbf{A} \in \mathrm{IR}^{n\times n} \text{ such that } \mathbf{u}(\mathbf{x}) = \mathbf{b} + \mathbf{A}\mathbf{x}\}, \end{aligned}$$

is the space of all infinitesimal rigid displacements. In X_2 we fix the freedom of $\mathbf{u}$ with respect to infinitesimal rigid displacements. With this notation a weak formulation of (2.9) and (2.10) can be written as

$$\langle \boldsymbol{\eta}, D_{\mathbf{u}}E(\mathbf{c},\mathbf{u})\rangle = 0 \text{ for all } \boldsymbol{\eta} \in X_2, \tag{3.3}$$

where $D_{\mathbf{u}}E$ is the derivative of E with respect to $\mathbf{u}$ in the space X_2. Since $W_{,\mathcal{E}}(\mathbf{c},\mathcal{E})$ is symmetric if $\mathcal{E}$ is symmetric we can also allow for arbitrary $\boldsymbol{\eta} \in H^1(\Omega, \mathrm{I\!R}^n)$ in (3.3).

We remark that the above discussion was of formal nature but can be justified rigorously under suitable conditions on Ψ, W, $\mathbf{c}$ and $\mathbf{u}$.

3.2. **Assumptions.** We state the following assumptions:

(A1) $\Omega \subset \mathrm{I\!R}^n$ is a bounded domain with Lipschitz boundary,
(A2) the gradient energy tensor $\boldsymbol{\Gamma}$ is a constant, symmetric, positive definite linear mapping of $\mathrm{I\!R}^{N\times n}$ into itself, i.e. in particular there exists a constant $\gamma_0 > 0$ such that

$$\mathbf{A}' : \boldsymbol{\Gamma}\mathbf{A}' \geq \gamma_0 |\mathbf{A}'|^2,$$

for all $\mathbf{A}' \in \mathrm{I\!R}^{N\times n}$,
(A3) the homogeneous free energy density Ψ can be written as

$$\Psi(\mathbf{c}') = \Psi^1(\mathbf{c}') + \Psi^2(\mathbf{c}') \quad \text{ for all } \mathbf{c}' \in \mathrm{I\!R}^N$$

with $\Psi^1, \Psi^2 \in C^1(\mathrm{I\!R}^N, \mathrm{I\!R})$ and Ψ^1 convex. In addition, we assume
(A3.1) $\Psi^1 \geq 0$,
(A3.2) for all $\delta > 0$ there exists a $C_\delta > 0$ such that

$$|\Psi^1_{,\mathbf{c}}(\mathbf{c}')| \leq \delta \Psi^1(\mathbf{c}') + C_\delta \text{ for all } \mathbf{c}' \in \Sigma,$$

(A3.3) there exists a constant $C_1 > 0$ such that

$$|\Psi^2_{,\mathbf{c}}(\mathbf{c}')| \leq C_1(|\mathbf{c}'| + 1) \text{ for all } \mathbf{c}' \in \Sigma,$$

(A4) for the elastic energy density $W \in C^1(\mathrm{I\!R}^N \times \mathrm{I\!R}^{n\times n}, \mathrm{I\!R})$ we assume
(A4.1) $W(\mathbf{c}', \mathcal{E}')$ only depends on the symmetric part of $\mathcal{E}' \in \mathrm{I\!R}^{n\times n}$, i.e. $W(\mathbf{c}', \mathcal{E}') = W(\mathbf{c}', (\mathcal{E}')^t)$ for all $\mathbf{c}' \in \mathrm{I\!R}^N$ and $\mathcal{E}' \in \mathrm{I\!R}^{n\times n}$,
(A4.2) $W_{,\mathcal{E}}(\mathbf{c}', .)$ is strongly monotone uniformly in $\mathbf{c}'$, i.e. there exists a $c_1 > 0$ such that for all symmetric $\mathcal{E}'_1, \mathcal{E}'_2 \in \mathrm{I\!R}^{n\times n}$

$$(W_{,\mathcal{E}}(\mathbf{c}', \mathcal{E}'_2) - W_{,\mathcal{E}}(\mathbf{c}', \mathcal{E}'_1)) : (\mathcal{E}'_2 - \mathcal{E}'_1) \geq c_1 |\mathcal{E}'_2 - \mathcal{E}'_1|^2,$$

(A4.3) there exists a constant $C_2 > 0$ such that for all $\mathbf{c}' \in \Sigma$ and all symmetric $\mathcal{E}' \in \mathrm{I\!R}^{n\times n}$

$$|W(\mathbf{c}', \mathcal{E}')| \leq C_2(|\mathcal{E}'|^2 + |\mathbf{c}'|^2 + 1),$$
$$|W_{,\mathbf{c}}(\mathbf{c}', \mathcal{E}')| \leq C_2(|\mathcal{E}'|^2 + |\mathbf{c}'|^2 + 1),$$
$$|W_{,\mathcal{E}}(\mathbf{c}', \mathcal{E}')| \leq C_2(|\mathcal{E}'| + |\mathbf{c}'| + 1),$$

(A5) the energy density of the applied forces is assumed to be of the form $W^*(\mathcal{E}') = -\mathcal{E}' : \mathcal{S}^*$ with a constant symmetric tensor $\mathcal{S}^*$,

(A6) the mobility matrix $\mathbf{L} = (L_{kl})_{k=1,\dots,N;l=1,\dots,N}$ is assumed to be

(A6.1) symmetric,

(A6.2) to fulfil $\sum_{l=1}^{N} L_{kl} = 0$,

(A6.3) to be positive definite on $T\Sigma$,

(A7) the initial data $\mathbf{c}^0 \in X_1$ are assumed to fulfil $\int_\Omega \Psi(\mathbf{c}^0) < \infty$.

Let us comment on the stated assumptions. The assumptions on $\mathbf{\Gamma}$ and $\mathbf{L}$ guarantee that the system (2.7), (2.8) defines a semi-linear parabolic system of fourth order in the variable $\mathbf{c}$. Assumption (A3) uses a splitting of the homogeneous free energy density Ψ. A convex part Ψ^1 is allowed to have large growth for $\mathbf{c}'$ large. We only assume that the derivative $\Psi^1_{,\mathbf{c}}$ can be controlled by Ψ^1 itself. Any polynomial growth for Ψ^1 is allowed. Note that for example an exponential growth in Ψ is not allowed and we remark that a growth larger than a polynomial growth could be treated with a method analogous to the one presented in Garcke [22]. The non-convex part Ψ^2 is allowed to grow such that $\Psi^2_{,\mathbf{c}}$ is sub-linear. The assumption (A4.1) guarantees that $W_{,\mathcal{E}}(\mathbf{c}, \mathcal{E}')$ is symmetric for all symmetric $\mathcal{E}' \in \mathbb{R}^{n\times n}$. The monotonicity (A4.2) ensures that the elastic part of the equation defines a quasi-linear elliptic system in $\mathcal{E}$. Since

$$W(\mathbf{c}', \mathcal{E}') = W(\mathbf{c}', \mathbf{0}) + \int_0^1 W_{,\mathcal{E}}(\mathbf{c}', t\mathcal{E}') : \mathcal{E}' dt$$

we can use assumptions (A4.2) and (A4.3) to conclude that there exist positive constants c_3 and C_3 such that

$$W(\mathbf{c}', \mathcal{E}') \geq c_3 |\mathcal{E}'|^2 - C_3 \left(|\mathbf{c}'|^2 + 1\right)$$

for all $\mathbf{c}' \in \Sigma$ and all symmetric $\mathcal{E}' \in \mathbb{R}^{n\times n}$.

In the existence proof we will formulate a variational problem whose Euler-Lagrange equations are an implicit time discretisation of the elliptic-parabolic system. The growth conditions on Ψ and W ensure existence of a solution to the variational problem and enables us to compute the corresponding Euler-Lagrange equations. We also note that it would be enough to state assumptions on $\mathbf{P}\Psi^1_{,\mathbf{c}}$, $\mathbf{P}\Psi^2_{,\mathbf{c}}$ and $\mathbf{P}W_{,\mathbf{c}}$ rather than $\Psi^1_{,\mathbf{c}}$, $\Psi^2_{,\mathbf{c}}$ and $W_{,\mathbf{c}}$. The evolution law is stated solely on Σ and hence Ψ and W can be chosen arbitrary in the direction orthogonal to Σ.

3.3. **Weak solutions.** The goal of Section 3 is to show existence of a weak solution to the problem (2.7)-(2.14). We will use the following solution concept. Let $T > 0$ be an arbitrary but fixed time and $\Omega_T := \Omega \times (0,T)$.

Definition 3.1. (Weak solution) *A triple* $(\mathbf{c}, \mathbf{w}, \mathbf{u}) \in L^2(0,T; H^1(\Omega, \mathbb{R}^N)) \times L^2(0,T; H^1(\Omega, \mathbb{R}^N)) \times L^2(0,T; X_2)$ *with* $\mathbf{P}\Psi_{,\mathbf{c}}(\mathbf{c}) \in L^1(\Omega_T)$ *is called a weak solution of (2.7)-(2.14) if and only if*
(i)

$$-\int_{\Omega_T} \partial_t \boldsymbol{\xi} \cdot (\mathbf{c} - \mathbf{c}^0) + \int_{\Omega_T} \mathbf{L} \nabla \mathbf{w} : \nabla \boldsymbol{\xi} = 0 \tag{3.4}$$

for all $\boldsymbol{\xi} \in L^2(0,T; H^1(\Omega, \mathbb{R}^N))$ *with* $\partial_t \boldsymbol{\xi} \in L^2(\Omega_T)$ *and* $\boldsymbol{\xi}(T) = 0$,
(ii)

$$\int_{\Omega_T} \mathbf{w} \cdot \boldsymbol{\zeta} = \int_{\Omega_T} \{ \boldsymbol{\Gamma} \nabla \mathbf{c} : \nabla \mathbf{P} \boldsymbol{\zeta} + \mathbf{P}\Psi_{,\mathbf{c}}(\mathbf{c}) \cdot \boldsymbol{\zeta} + \mathbf{P} W_{,\mathbf{c}}(\mathbf{c}, \mathcal{E}(\mathbf{u})) \cdot \boldsymbol{\zeta} \} \tag{3.5}$$

for all $\boldsymbol{\zeta} \in L^2(0,T; H^1(\Omega, \mathbb{R}^N)) \cap L^\infty(\Omega_T, \mathbb{R}^N)$, *and*
(iii)

$$\int_{\Omega_T} W_{,\mathcal{E}}(\mathbf{c}, \mathcal{E}(\mathbf{u})) : \nabla \boldsymbol{\eta} = \int_{\Omega_T} \mathcal{S}^* : \nabla \boldsymbol{\eta} \tag{3.6}$$

for all $\boldsymbol{\eta} \in L^2(0,T; H^1(\Omega, \mathbb{R}^n))$.

Now let us state the existence theorem that will be proved in the following subsections.

Theorem 3.1. *Assume (A1)-(A7). Then there exists a weak solution in the sense of Definition 3.1 which has the following properties:*
(i) $\mathbf{c} \in C^{0,\frac{1}{4}}([0,T]; L^2(\Omega))$,
(ii) $\partial_t \mathbf{c} \in L^2\left(0,T; (H^1(\Omega))^*\right)$,
(iii) $\mathbf{u} \in L^\infty\left(0,T; H^1(\Omega, \mathbb{R}^n)\right)$.

Remark 3.1. *Using arguments of Garcke* [22] *it is possible to show higher integrability of* $\nabla \mathbf{u}$, *i.e. there exists a* $p > 2$ *such that* $\nabla \mathbf{u} \in L^\infty\left(0,T; L^p(\Omega, \mathbb{R}^n)\right)$. *In two space dimensions this and the Sobolev embedding then implies that* $\mathbf{u} \in L^\infty\left(0,T; C^{0,\alpha}(\Omega, \mathbb{R}^2)\right)$ *for some* $\alpha > 0$.

3.4. **The implicit time discretisation.** For $T > 0$ and $M \in \mathbb{N}$ we define $\Delta t = \frac{T}{M}$. Then an implicit time discretisation of the system

(2.7)-(2.10) is given by

$$\begin{aligned} \frac{\mathbf{c}^m - \mathbf{c}^{m-1}}{\Delta t} &= \mathbf{L}\Delta \mathbf{w}^m, && (3.7)\\ \mathbf{w}^m &= \mathbf{P}\left(-\nabla\cdot\mathbf{\Gamma}\nabla\mathbf{c}^m + \Psi_{,\mathbf{c}}(\mathbf{c}^m) + W_{,\mathbf{c}}(\mathbf{c}^m,\mathcal{E}^m)\right), && (3.8)\\ \nabla\cdot\mathcal{S}^m &= 0, && (3.9)\\ \mathcal{S}^m &= W_{,\mathcal{E}}(\mathbf{c}^m,\mathcal{E}^m), && (3.10)\end{aligned}$$

for $(\mathbf{c}^m, \mathbf{w}^m, \mathbf{u}^m)$. By an upper index $m \in \{0, ..., M\}$ we denote the time discrete solution at time $m\Delta t$ and $\mathcal{E}^m$ is an abbreviation for $\mathcal{E}(\mathbf{u}^m)$.

Assuming that $\mathbf{c}^0 \in X_1$ is given we want to determine $(\mathbf{c}^m, \mathbf{w}^m, \mathbf{u}^m)$ and hence $\mathcal{S}^m$ inductively by solving (3.7)-(3.10) together with the boundary conditions (2.11)-(2.13) for $(\mathbf{c}^m, \mathbf{w}^m, \mathbf{u}^m)$.

Analogously to the discussion leading to (3.2) one can derive

$$\langle \boldsymbol{\zeta}, D_{\mathbf{c}}E(\mathbf{c}^m,\mathbf{u}^m)\rangle = -\left(\boldsymbol{\zeta}, \frac{\mathbf{c}^m-\mathbf{c}^{m-1}}{\Delta t}\right)_{\mathbf{L}} \text{ for all } \boldsymbol{\zeta}\in Y. \qquad (3.11)$$

Also we have

$$\langle \boldsymbol{\eta}, D_{\mathbf{u}}E(\mathbf{c}^m,\mathbf{u}^m)\rangle = 0 \text{ for all } \boldsymbol{\eta}\in X_2 \qquad (3.12)$$

and we observe that (3.11) and (3.12) are the Euler-Lagrange equations of the functional

$$E^{m,\Delta t}(\mathbf{d},\mathbf{v}) := E(\mathbf{d},\mathbf{v}) + \tfrac{1}{2\Delta t}\|\mathbf{d}-\mathbf{c}^{m-1}\|^2_{\mathbf{L}}. \qquad (3.13)$$

Our goal now is to show the existence of an absolute minimiser of $E^{m,\Delta t}$ in the class $X_1^{\mathbf{m}} \times X_2$ where $\mathbf{m} := \fint_\Omega \mathbf{c}^0$.

Lemma 3.1. *Assume (A1)-(A6) and suppose* $\mathbf{c}^{m-1} \in X_1^{\mathbf{m}}$.

Then there exists a minimiser of $E^{m,\Delta t}$ *in* $X_1^{\mathbf{m}} \times X_2$ *provided that* $\Delta t \in \left(0, \frac{\gamma_0}{8(C_1+C_3)^2 C_{\mathbf{L}}}\right)$.

Proof. The existence of a minimiser can be shown by the direct method. We outline the main steps. Using the assumptions (A2)-(A6) we deduce that there exists a constant $C > 0$ such that for all $(\mathbf{d},\mathbf{v}) \in X_1^{\mathbf{m}} \times X_2$

$$\begin{aligned} &E^{m,\Delta t}(\mathbf{d},\mathbf{v}) \geq \\ &\tfrac{\gamma_0}{2}\|\nabla\mathbf{d}\|^2_{L^2} + \tfrac{c_3}{2}\|\mathcal{E}(\mathbf{v})\|^2_{L^2} + \tfrac{1}{2\Delta t}\|\mathbf{d}-\mathbf{c}^{m-1}\|^2_{\mathbf{L}} - (C_3+C_1)\|\mathbf{d}\|^2_{L^2} - C.\end{aligned}$$

We remark that in this paper C denotes any positive constant depending on known quantities. The value of C may change from line to line in a given computation. Since $\mathbf{d} - \mathbf{c}^{m-1} \in Y$ we can use (3.1) and the fact that $\mathbf{c}^{m-1}$ is bounded in $H^1(\Omega, \mathbb{R}^N)$ to conclude

$$\begin{aligned}E^{m,\Delta t}(\mathbf{d},\mathbf{v}) \geq \left(\tfrac{\gamma_0}{2} - (C_1 + C_3)\delta\right) \|\nabla \mathbf{d}\|^2_{L^2} + \\ + \tfrac{c_2}{2}\|\mathcal{E}(\mathbf{v})\|^2_{L^2} + \left(\tfrac{1}{2\Delta t} - \tfrac{(C_1+C_3)C_{\mathbf{L}}}{\delta}\right) \|\mathbf{d} - \mathbf{c}^{m-1}\|^2_{\mathbf{L}} - C\end{aligned}$$

where C depends on $\mathbf{c}^{m-1}$. Since we assumed $\Delta t < \frac{\gamma_0}{8(C_1+C_3)^2 C_{\mathbf{L}}}$ we can choose $\delta = \frac{\gamma_0}{4(C_1+C_3)}$ and obtain with the help of inequalities of Korn (Theorem 5.2) and Poincaré, that $E^{m,\Delta t}$ is coercive on the space $X_1^{\mathbf{m}} \times X_2$.

The space $X_1^{\mathbf{m}} \times X_2$ is non-empty and hence we can choose a minimising sequence $(\mathbf{d}_\kappa, \mathbf{v}_\kappa)_{\kappa \in \mathbb{N}}$ with

$$\infty > E^{m,\Delta t}(\mathbf{d}_\kappa, \mathbf{v}_\kappa) \to \inf_{(\mathbf{d},\mathbf{v}) \in X_1^{\mathbf{m}} \times X_2} E^{m,\Delta t}(\mathbf{d}, \mathbf{v}).$$

The coercivity of $E^{m,\Delta t}$ implies that $\{(\mathbf{d}_\kappa, \mathbf{v}_\kappa)\}_{\kappa \in \mathbb{N}}$ is uniformly bounded in $X_1^{\mathbf{m}} \times X_2$. Without loss of generality we can assume that $\{(\mathbf{d}_\kappa, \mathbf{v}_\kappa)\}_{\kappa \in \mathbb{N}}$ converges weakly in $X_1^{\mathbf{m}} \times X_2$ to a limit $(\mathbf{d}, \mathbf{v})$ (otherwise we replace the original sequence by a converging subsequence). Furthermore, we can assume that $\mathbf{d}_\kappa$ converges strongly in $L^2(\Omega, \mathbb{R}^N)$ and almost everywhere in Ω.

All terms in the energy besides $\int_\Omega \Psi^2(\mathbf{d})$ and $\int_\Omega W(\mathbf{d}, \mathcal{E}(\mathbf{u}))$ are convex and therefore sequentially weakly lower semi-continuous on $X_1^{\mathbf{m}} \times X_2$. Let us now discuss the remaining two terms. Condition (A3.3) implies that $\Psi^2(\mathbf{c}')$ has at most a quadratic growth for large $\mathbf{c}' \in \Sigma$ and hence the generalised dominated convergence theorem (see e.g. [1, 46]) of Lebesgue yields: $\int_\Omega \Psi^2(\mathbf{d}_\kappa) \to \int_\Omega \Psi^2(\mathbf{d})$. It remains to show

$$\int_\Omega W(\mathbf{d}, \mathcal{E}(\mathbf{v})) \leq \liminf_{\kappa \to \infty} \int_\Omega W(\mathbf{d}_\kappa, \mathcal{E}(\mathbf{v}_\kappa)). \tag{3.14}$$

Using the convexity of $W(\mathbf{c}', .)$ (which follows from (A4.2)) we have

$$\begin{aligned}&\int_\Omega \{W(\mathbf{d}_\kappa, \mathcal{E}(\mathbf{v}_\kappa)) - W(\mathbf{d}, \mathcal{E}(\mathbf{v}))\} = \\ &= \int_\Omega \{W(\mathbf{d}_\kappa, \mathcal{E}(\mathbf{v}_\kappa)) - W(\mathbf{d}_\kappa, \mathcal{E}(\mathbf{v}))\} + \int_\Omega \{W(\mathbf{d}_\kappa, \mathcal{E}(\mathbf{v})) - W(\mathbf{d}, \mathcal{E}(\mathbf{v}))\} \\ &\geq \int_\Omega \{W_{,\mathcal{E}}(\mathbf{d}_\kappa, \mathcal{E}(\mathbf{v})) : (\mathcal{E}(\mathbf{v}_\kappa) - \mathcal{E}(\mathbf{v}))\} + \int_\Omega \{W(\mathbf{d}_\kappa, \mathcal{E}(\mathbf{v})) - W(\mathbf{d}, \mathcal{E}(\mathbf{v}))\}.\end{aligned}$$

The weak convergence of $\mathcal{E}(\mathbf{v}_\kappa)$ in L^2, the strong convergence of $\mathbf{d}_\kappa$ in L^2, the convergence almost everywhere of $\mathbf{d}_\kappa$ and the growth conditions in (A4.3) then give (3.14). This yields

$$E^{m,\Delta t}(\mathbf{d}, \mathbf{v}) \leq \liminf_{\kappa \to \infty} E^{m,\Delta t}(\mathbf{d}_\kappa, \mathbf{v}_\kappa)$$

and implies that $(\mathbf{d}, \mathbf{v})$ minimises $E^{m,\Delta t}$ in $X_1^{\mathbf{m}} \times X_2$. $\square$

From now on we assume that Δt is small enough for a minimum to exist. We choose the value at the new time step $(\mathbf{c}^m, \mathbf{u}^m)$ as a minimiser of $E^{m,\Delta t}$. In the following lemma we compute the Euler-Lagrange equation associated with $E^{m,\Delta t}$ which hold for $(\mathbf{c}^m, \mathbf{u}^m)$.

Lemma 3.2. (Euler-Lagrange equations) *The minimiser* $(\mathbf{c}^m, \mathbf{u}^m)$ *fulfils*
(i)

$$\int_\Omega \left(\frac{\mathbf{c}^m - \mathbf{c}^{m-1}}{\Delta t}\right) \cdot \boldsymbol{\xi} + \int_\Omega \mathbf{L}\nabla \mathbf{w}^m : \nabla \boldsymbol{\xi} = 0 \tag{3.15}$$

for all $\boldsymbol{\xi} \in H^1(\Omega, \mathrm{I\!R}^N)$.
(ii)

$$\int_\Omega \mathbf{w}^m \cdot \boldsymbol{\zeta} = \int_\Omega \{\boldsymbol{\Gamma}\nabla \mathbf{u}^m : \nabla \mathbf{P}\boldsymbol{\zeta} + \mathbf{P}\Psi_{,\mathbf{c}}(\mathbf{c}^m) \cdot \boldsymbol{\zeta} + \mathbf{P}W_{,\mathbf{c}}(\mathbf{c}^m, \mathbf{u}^m) \cdot \boldsymbol{\zeta}\} \tag{3.16}$$

for all $\boldsymbol{\zeta} \in L^\infty(\Omega, \mathrm{I\!R}^N) \cap H^1(\Omega, \mathrm{I\!R}^N)$.
(iii)

$$\int_\Omega W_{,\mathcal{E}}(\mathbf{c}^m, \mathcal{E}(\mathbf{u}^m)) : \nabla \boldsymbol{\eta} = \int_\Omega \mathcal{S}^* : \nabla \boldsymbol{\eta} \tag{3.17}$$

for all $\boldsymbol{\eta} \in H^1(\Omega, \mathrm{I\!R}^n)$.

Here, $\mathbf{w}^m = \mathcal{G}\left(\frac{\mathbf{c}^m - \mathbf{c}^{m-1}}{\Delta t}\right) + \boldsymbol{\lambda}^m \in H^1(\Omega, \mathrm{I\!R}^N)$ *where*

$$\boldsymbol{\lambda}^m = \fint_\Omega \left\{\mathbf{P}\Psi_{,\mathbf{c}}(\mathbf{c}^m) + \mathbf{P}W_{,\mathbf{c}}(\mathbf{c}^m, \mathcal{E}(\mathbf{u}^m))\right\}$$

is a constant Lagrange multiplier. Furthermore, it holds $\mathbf{P}\mathbf{w}^m = \mathbf{w}^m$.

Proof. We choose $\boldsymbol{\zeta} \in L^\infty(\Omega, \mathrm{I\!R}^N) \cap Y$, $\boldsymbol{\eta} \in X_2$ and want to determine

$$\lim_{\varepsilon \to 0} \frac{E^{m,\Delta t}(\mathbf{c}^m + \varepsilon\boldsymbol{\zeta}, \mathbf{u}^m + \varepsilon\boldsymbol{\eta}) - E^{m,\Delta t}(\mathbf{c}^m, \mathbf{u}^m)}{\varepsilon}. \tag{3.18}$$

Since Ψ^1 is convex, it holds

$$\Psi^1(\mathbf{c}^m) \geq \Psi^1(\mathbf{c}^m + \varepsilon\boldsymbol{\zeta}) - \varepsilon\Psi^1_{,\mathbf{c}}(\mathbf{c}^m + \varepsilon\boldsymbol{\zeta}) \cdot \boldsymbol{\zeta}$$

which implies by Assumption (A3.2) that

$$\begin{aligned} \Psi^1(\mathbf{c}^m + \varepsilon\boldsymbol{\zeta}) &\leq \Psi^1(\mathbf{c}^m) + |\varepsilon\mathbf{P}\Psi^1_{,\mathbf{c}}(\mathbf{c}^m + \varepsilon\boldsymbol{\zeta})| \|\boldsymbol{\zeta}\|_{L^\infty} \\ &\leq \Psi^1(\mathbf{c}^m) + |\varepsilon|\Psi^1(\mathbf{c}^m + \varepsilon\boldsymbol{\zeta})\|\boldsymbol{\zeta}\|_{L^\infty} + C|\varepsilon|. \end{aligned}$$

Hence, for ε small we obtain

$$\left(\Psi^1(\mathbf{c}^m + \varepsilon\boldsymbol{\zeta}) + |\mathbf{P}\Psi^1_{,\mathbf{c}}(\mathbf{c}^m + \varepsilon\boldsymbol{\zeta})|\right) \leq C\left(\Psi^1(\mathbf{c}^m) + 1\right)$$

and therefore,

$$\left|\frac{\Psi^1(\mathbf{c}^m+\varepsilon\boldsymbol{\zeta})-\Psi^1(\mathbf{c}^m)}{\varepsilon}\right| \le C(\Psi^1(\mathbf{c}^m)+1).$$

The dominated convergence theorem of Lebesgue and Assumption (A3.3) yield

$$\lim_{\varepsilon\to 0}\tfrac{1}{\varepsilon}\left(\int_\Omega \Psi(\mathbf{c}^m+\varepsilon\boldsymbol{\zeta})-\Psi(\mathbf{c}^m)\right)=\int_\Omega \Psi_{,\mathbf{c}}(\mathbf{c}^m)\cdot\boldsymbol{\zeta}.$$

Using the growth condition (A4.3) we compute

$$\begin{aligned}\lim_{\varepsilon\to 0}&\int_\Omega \tfrac{1}{\varepsilon}\left(W\left(\mathbf{c}^m+\varepsilon\boldsymbol{\zeta},\mathcal{E}(\mathbf{u}^m+\varepsilon\boldsymbol{\eta})\right)-W\left(\mathbf{c}^m,\mathcal{E}(\mathbf{u}^m)\right)\right)\\ &=\int_\Omega \left(W_{,\mathbf{c}}(\mathbf{c}^m,\mathcal{E}(\mathbf{u}^m))\boldsymbol{\zeta}+W_{,\mathcal{E}}(\mathbf{c}^m,\mathcal{E}(\mathbf{u}^m)):\nabla\boldsymbol{\eta}\right). \qquad (3.19)\end{aligned}$$

Since the term $\frac{1}{2\Delta t}\|\mathbf{d}-\mathbf{c}^{m-1}\|^2_{\mathbf{L}}$ is quadratic we obtain

$$\begin{aligned}\lim_{\varepsilon\to 0}\tfrac{1}{\varepsilon}\tfrac{1}{2\Delta t}&\left(\|(\mathbf{c}^m+\varepsilon\boldsymbol{\zeta})-\mathbf{c}^{m-1}\|^2_{\mathbf{L}}-\|\mathbf{c}^m-\mathbf{c}^{m-1}\|^2_{\mathbf{L}}\right)\\ &=\left(\frac{\mathbf{c}^m-\mathbf{c}^{m-1}}{\Delta t},\boldsymbol{\zeta}\right)_{\mathbf{L}}\\ &=\left(\mathcal{G}\left(\frac{\mathbf{c}^m-\mathbf{c}^{m-1}}{\Delta t}\right),\boldsymbol{\zeta}\right)_{L^2}.\end{aligned}$$

Since

$$\mathbf{w}^m=\mathcal{G}\left(\frac{\mathbf{c}^m-\mathbf{c}^{m-1}}{\Delta t}\right)+\boldsymbol{\lambda}^m$$

and

$$\boldsymbol{\lambda}^m=\fint_\Omega\left(\mathbf{P}\Psi_{,\mathbf{c}}(\mathbf{c}^m)+\mathbf{P}W_{,\mathbf{c}}(\mathbf{c}^m,\mathcal{E}(\mathbf{u}^m))\right)$$

we obtain (3.15) taking into account that $\mathbf{w}^m$ and $\mathbf{c}^m-\mathbf{c}^{m-1}$ attain values in $T\Sigma$ almost everywhere. The identity (3.16) follows from the above computations for all $\boldsymbol{\zeta}\in L^\infty(\Omega,\mathrm{I\!R}^N)\cap Y$ since (3.18) is equal to zero for the minimiser $(\mathbf{c}^m,\mathbf{u}^m)$. For arbitrary $\boldsymbol{\zeta}\in L^\infty(\Omega,\mathrm{I\!R}^N)\cap H^1(\Omega,\mathrm{I\!R}^N)$ equation (3.16) follows because of the definition of $\boldsymbol{\lambda}^m$ and since $\mathbf{P}\mathbf{w}^m=\mathbf{w}^m$.

The identity (3.17) follows for all $\boldsymbol{\eta}\in X_2$ from varying $E^{m,\Delta t}$ with respect to $\mathbf{u}$. For arbitrary $\boldsymbol{\eta}\in H^1(\Omega,\mathrm{I\!R}^n)$ we obtain (3.17) since $W_{,\mathcal{E}}$ and $\mathcal{S}^*$ are symmetric. $\square$

3.5. **Uniform estimates.** So far we determined solutions $(\mathbf{c}^m, \mathbf{u}^m)$ and related generalised chemical potential differences $\mathbf{w}^m$ $(m = 1, ..., M)$ for every fixed $M \in \mathbb{N}$. Now we define the piecewise constant extension $(\mathbf{c}_M, \mathbf{w}_M, \mathbf{u}_M)$ of $\{(\mathbf{c}^m, \mathbf{w}^m, \mathbf{u}^m)\}_{m=1,...,M}$. For $t \in ((m-1)\Delta t, m\Delta t]$ we set

$$(\mathbf{c}_M, \mathbf{w}_M, \mathbf{u}_M)(\cdot, t) := (\mathbf{c}^m_M, \mathbf{w}^m_M, \mathbf{u}^m_M)(\cdot) := (\mathbf{c}^m, \mathbf{w}^m, \mathbf{u}^m)(\cdot).$$

The piecewise linear extension $(\bar{\mathbf{c}}_M, \bar{\mathbf{w}}_M, \bar{\mathbf{u}}_M)$ of $\{(\mathbf{c}^m, \mathbf{w}^m, \mathbf{u}^m)\}_{m=1,...,M}$ is defined for $t = \beta m\Delta t + (1-\beta)(m-1)\Delta t$ with $\beta \in [0, 1]$ as

$$(\bar{\mathbf{c}}_M, \bar{\mathbf{w}}_M, \bar{\mathbf{u}}_M)(\cdot, t) := \beta(\mathbf{c}^m_M, \mathbf{w}^m_M, \mathbf{u}^m_M)(\cdot) + (1-\beta)(\mathbf{c}^{m-1}_M, \mathbf{w}^{m-1}_M, \mathbf{u}^{m-1}_M)(\cdot).$$

In order to derive a priori estimates we show a discrete version of the dissipation inequality (2.15) for the time discrete solutions.

Lemma 3.3. *Assume (A1)-(A7). Then the following a priori estimates hold.*
a) For all $M \in \mathbb{N}$ and $t \in [0, T]$ we have

$$E(\mathbf{c}_M(t), \mathbf{u}_M(t)) + \tfrac{1}{2}\int_{\Omega_t} \mathbf{L}\nabla\mathbf{w}_M : \nabla\mathbf{w}_M \le E(\mathbf{c}^0, \mathbf{u}^0).$$

Here, $\mathbf{u}^0$ is chosen to be the minimiser of $\mathbf{v} \mapsto \int_\Omega \{W(\mathbf{c}^0, \mathcal{E}(\mathbf{v})) + W^*(\mathcal{E}(\mathbf{v}))\}$ in the class X_2.
b) There exists a constant $C > 0$ such that

$$\sup_{t\in[0,T]} \left\{\|\mathbf{c}_M(t)\|_{H^1(\Omega)} + \|\mathbf{u}_M(t)\|_{H^1(\Omega)}\right\} \le C \tag{3.20}$$

and

$$\sup_{t\in[0,T]} \int_\Omega \{\Psi^1(\mathbf{c}_M(t)) + \|\nabla\mathbf{w}_M\|_{L^2(\Omega_T)}\} \le C. \tag{3.21}$$

Proof. Taking $(\mathbf{c}^{m-1}_M, \mathbf{u}^{m-1}_M)$ as a comparison function when minimising (3.13) we obtain

$$E(\mathbf{c}^m_M, \mathbf{u}^m_M) + \tfrac{1}{2\Delta t}\|\mathbf{c}^m_M - \mathbf{c}^{m-1}_M\|^2_{\mathbf{L}} \le E(\mathbf{c}^{m-1}_M, \mathbf{u}^{m-1}_M).$$

Using this inequality iteratively and using the definitions of the product $(.,.)_{\mathbf{L}}$ and of $\mathbf{w}^m_M$ gives for all $M \in \mathbb{N}$ and $m \in \{1, ..., M\}$

$$E(\mathbf{c}^m_M, \mathbf{u}^m_M) + \tfrac{1}{2}\int_0^{m\Delta t} (\mathbf{L}\nabla\mathbf{w}^m_M, \nabla\mathbf{w}^m_M)_{L^2} \le E(\mathbf{c}^0, \mathbf{u}^0).$$

Due to $⨍ \mathbf{c}^m_M = \mathbf{m}$ and $\mathbf{u}^m_M \in X_2$ we can use Assumptions (A2)-(A7) and the inequalities of Poincaré and Korn to conclude (3.20) and (3.21) $\square$

Since $\bar{\mathbf{c}}_M$ is the piecewise linear interpolant of the $\mathbf{c}_M^m$ we can rewrite (3.15) as

$$\int_\Omega \partial_t \bar{\mathbf{c}}_M \cdot \boldsymbol{\xi} + \int_\Omega \mathbf{L}\nabla \mathbf{w}_M : \nabla \boldsymbol{\xi} = 0 \text{ for all } \boldsymbol{\xi} \in H^1(\Omega, \mathbb{R}^N), \qquad (3.22)$$

which holds for almost all $t \in (0,T)$. This identity together with the estimates in Lemma 3.3 enables us to control time differences of $\bar{\mathbf{c}}_M$ and $\mathbf{c}_M$.

Lemma 3.4. *There exists a constant $C > 0$ such that for all $t_1, t_2 \in [0,T]$*

$$\|\bar{\mathbf{c}}_M(t_2) - \bar{\mathbf{c}}_M(t_1)\|_{L^2(\Omega)} \le C|t_2 - t_1|^{\frac{1}{4}}.$$

Furthermore, we can choose a subsequence $\{\mathbf{c}_M\}_{M\in\mathcal{N}}$ with $\mathcal{N} \subset \mathbb{N}$ and a $\mathbf{c} \in L^\infty(0,T;H^1(\Omega))$ such that for all $\alpha \in (0, \frac{1}{4})$

$$\begin{array}{lrcl}
(i) & \bar{\mathbf{c}}_M & \to & \mathbf{c} \textit{ in } C^{0,\alpha}([0,T]; L^2(\Omega)),\\
(ii) & \mathbf{c}_M & \to & \mathbf{c} \textit{ in } L^\infty(0,T; L^2(\Omega)),\\
(iii) & \mathbf{c}_M & \to & \mathbf{c} \textit{ almost everywhere in } \Omega_T,\\
(iv) & \nabla\mathbf{c}_M & \to & \nabla\mathbf{c} \textit{ weak-* in } L^\infty(0,T; L^2(\Omega)),\\
(v) & \Psi_{,\mathbf{c}}(\mathbf{c}_M) & \to & \Psi_{,\mathbf{c}}(\mathbf{c}) \textit{ in } L^1(\Omega_T),
\end{array}$$

as $M \in \mathcal{N}$ tends to infinity.

Proof. We choose $t_1, t_2 \in \mathbb{R}$ with $t_1 < t_2$ and $\boldsymbol{\xi} = \bar{\mathbf{c}}_M(t_2) - \bar{\mathbf{c}}_M(t_1)$ as a test function in (3.22) and integrate from t_1 to t_2 (compare [2]). This gives

$$\|\bar{\mathbf{c}}_M(t_2) - \bar{\mathbf{c}}_M(t_1)\|^2_{L^2(\Omega)} + \int_{t_1}^{t_2}\int_\Omega \mathbf{L}\nabla\mathbf{w}_M : \nabla(\bar{\mathbf{c}}_M(t_2) - \bar{\mathbf{c}}_M(t_1))dt = 0.$$

Since the $\mathbf{c}_M^m$ are uniformly bounded in $H^1(\Omega, \mathbb{R}^N)$ we obtain that the $\bar{\mathbf{c}}_M$ are uniformly bounded in $L^\infty(0,T;H^1(\Omega,\mathbb{R}^N))$. Hence,

$$\begin{aligned}
\|\bar{\mathbf{c}}_M(t_2) - \bar{\mathbf{c}}_M(t_1)\|^2_{L^2(\Omega)} &\le \\
&\le C\|\bar{\mathbf{c}}_M\|_{L^\infty(0,T;H^1(\Omega,\mathbb{R}^N))}\int_{t_1}^{t_2}\|\nabla\mathbf{w}_M\|_{L^2(\Omega)}(\tau)d\tau\\
&\le C\|\bar{\mathbf{c}}_M\|_{L^\infty(0,T;H^1(\Omega,\mathbb{R}^N))}(t_2-t_1)^{\frac{1}{2}}\|\nabla\mathbf{w}_M\|_{L^2(\Omega_T)}.
\end{aligned}$$

This implies the existence of a $C > 0$ such that

$$\|\bar{\mathbf{c}}_M(t_2) - \bar{\mathbf{c}}_M(t_1)\|_{L^2(\Omega)} \le C|t_2 - t_1|^{\frac{1}{4}} \qquad (3.23)$$

for all $t_1, t_2 \in [0,T]$.

Since $\{\bar{\mathbf{c}}_M\}_{M\in\mathbb{N}}$ is uniformly bounded in $L^\infty(0,T;H^1(\Omega,\mathbb{R}^N))$ and since the embedding from $H^1(\Omega,\mathbb{R}^N)$ into $L^2(\Omega,\mathbb{R}^N)$ is compact we can use the equicontinuity of $\{\bar{\mathbf{c}}_M\}_{M\in\mathbb{N}}$ (see (3.23)) to apply the theorem of Arzelà-Ascoli for functions with values in a Banach space (see Theorem 5.3). Hence, there exists a $\mathbf{c}$ such that (possibly along a subsequence)

$$\bar{\mathbf{c}}_M \to \mathbf{c} \qquad \text{in} \qquad C^{0,\alpha}(0,T;L^2(\Omega))$$

for all $\alpha \in (0, \frac{1}{4})$.

Choosing for $t \in [0,T]$ values $m \in \{1,...,M\}$ and $\beta \in [0,1]$ such that $t = \beta m \Delta t + (1-\beta)(m-1)\Delta t$ we obtain

$$\begin{aligned}
\|\bar{\mathbf{c}}_M(t) - \mathbf{c}_M(t)\|_{L^2} &= \|\beta \mathbf{c}_M^m + (1-\beta)\mathbf{c}_M^{m-1} - \mathbf{c}_M^m\|_{L^2} \\
&= (1-\beta)\|\mathbf{c}_M^m - \mathbf{c}_M^{m-1}\|_{L^2} \\
&\leq C(\Delta t)^{\frac{1}{4}}
\end{aligned}$$

which tends to zero as M tends to infinity. Together with (i) this implies (ii). In particular, we obtain that $\mathbf{c}_M$ converges in $L^2(\Omega_T)$. Therefore, we can extract a subsequence which converges almost everywhere. This shows (iii). The existence of a subsequence fulfilling (iv) follows from the boundedness of $\mathbf{c}_M$ in $L^\infty(0,T;H^1(\Omega))$ (see (3.20)).

It remains to show (v). The continuity of $\Psi_{,\mathbf{c}}$ and (iii) imply

$$\Psi_{,\mathbf{c}}(\mathbf{c}_M) \to \Psi_{,\mathbf{c}}(\mathbf{c})$$

almost everywhere. Using Assumption (A3.2) we get for all δ and all measurable sets $E \subset \Omega$

$$\begin{aligned}
\int_E |\Psi^1_{,\mathbf{c}}(\mathbf{c}_M)| &\leq \delta \int_E \Psi^1(\mathbf{c}_M) + C_\delta |E| \\
&\leq \delta C + C_\delta |E|.
\end{aligned}$$

Hence, $\int_E |\Psi^1_{,\mathbf{c}}(\mathbf{c}_M)|$ converges to zero uniformly in M as $|E|$ tends to zero. Employing the convergence theorem of Vitali (see [1, 46]) we have $\Psi^1_{,\mathbf{c}}(\mathbf{c}_M) \to \Psi^1_{,\mathbf{c}}(\mathbf{c})$ in $L^1(\Omega_T)$. The growth condition (A3.3) and Lebesgue's theorem yields the convergence of $\Psi^2_{,\mathbf{c}}(\mathbf{c}_M)$. This completes the proof of the lemma. □

We proceed in showing compactness in $\{\mathbf{u}_M\}_{M\in\mathbb{N}}$ and $\{\mathbf{w}_M\}_{M\in\mathbb{N}}$. In general $\mathcal{E}(\mathbf{u}_M)$ enters the equation for the chemical potential differences quadratically. Therefore, we will need strong convergence of $\{\nabla \mathbf{u}_M\}_M$ in $L^2(\Omega_T)$.

Lemma 3.5. *There exist subsequences $(\mathbf{u}_M)_{M\in\mathcal{N}}$, $(\mathbf{w}_M)_{M\in\mathcal{N}}$ with $\mathcal{N} \subset \mathbb{N}$ and $\mathbf{u} \in L^\infty(0,T;H^1(\Omega))$, $\mathbf{w} \in L^2(0,T;H^1(\Omega))$ such that*

$$\mathbf{u}_M \to \mathbf{u} \textit{ in } L^2(0,T;H^1(\Omega))$$

and

$$\mathbf{w}_M \to \mathbf{w} \textit{ weakly in } L^2(0,T;H^1(\Omega))$$

as $M \in \mathcal{N}$ tends to infinity,

PROOF. The estimate (3.20) and Korn's inequality (see Theorem 5.2) imply the existence of a subsequence such that

$$\mathbf{u}_M \to \mathbf{u} \text{ weakly in } L^2(0,T;H^1(\Omega))$$

for a $\mathbf{u} \in L^2(0,T;X_2)$. Choosing $\boldsymbol{\eta} = (\mathbf{u}_M - \mathbf{u})(t)$ for $t \in ((m-1)\Delta t, m\Delta t)$ as a test function in (3.17) yields for almost all $t \in [0,T]$

$$\int_\Omega \left(W_{,\mathcal{E}}(\mathbf{c}_M, \mathcal{E}(\mathbf{u}_M)) : \nabla(\mathbf{u}_M - \mathbf{u})\right)(t) = \int_\Omega \left(\mathcal{S}^* : \nabla(\mathbf{u}_M - \mathbf{u})\right)(t).$$

Integrating in time from 0 to T, taking into account the symmetry of $W_{,\mathcal{E}}$ and $\mathcal{S}^*$ and using the monotonicity of $W_{,\mathcal{E}}$ we can deduce

$$\begin{aligned} c_1 \; & \|\mathcal{E}(\mathbf{u}_M - \mathbf{u})\|^2_{L^2(\Omega_T)} \\ & \leq \int_{\Omega_T} \left(W_{,\mathcal{E}}(\mathbf{c}_M, \mathcal{E}(\mathbf{u}_M)) - W_{,\mathcal{E}}(\mathbf{c}_M, \mathcal{E}(\mathbf{u}))\right) : \mathcal{E}(\mathbf{u}_M - \mathbf{u}) \\ & = -\int_{\Omega_T} W_{,\mathcal{E}}(\mathbf{c}_M, \mathcal{E}(\mathbf{u})) : \mathcal{E}(\mathbf{u}_M - \mathbf{u}) + \int_{\Omega_T} \mathcal{S}^* : \mathcal{E}(\mathbf{u}_M - \mathbf{u}). \end{aligned}$$

Now we can show that the right hand side converges to zero. To conclude this we use the growth condition on $W_{,\mathcal{E}}$, the convergence of $\{\mathbf{c}_M\}_{M\in\mathbb{N}}$ in $L^2(\Omega_T)$ and the weak convergence of $\{\mathbf{u}_M\}_{M\in\mathbb{N}}$ in $L^2(0,T;H^1(\Omega))$. Hence, $\|\mathcal{E}(\mathbf{u}_M - \mathbf{u})\|_{L^2(\Omega_T)}$ converges to zero and then Korn's inequality (see Theorem 5.2) implies strong convergence of $\{\mathbf{u}_M\}_{M\in\mathbb{N}}$ in $L^2(0,T;H^1(\Omega))$.

Estimate (3.21) yields a uniform bound of $\nabla \mathbf{w}_M$ in $L^2(\Omega_T)$. Also we know that for all $t \in [0,T]$

$$\fint_\Omega \mathbf{w}_M(t) = \boldsymbol{\lambda}_M(t) = \fint_\Omega \left(\mathbf{P}\Psi_{,\mathbf{c}}(\mathbf{c}^m) + \mathbf{P}W_{,\mathbf{c}}(\mathbf{c}^m, \mathcal{E}(\mathbf{u}^m))\right).$$

Taking assumptions (A3) and (A4) into account we conclude that the right hand side is uniformly bounded. By the generalised Poincaré inequality we infer that $\mathbf{w}_M$ is uniformly bounded in $L^2(0,T;H^1(\Omega))$. This shows the existence of a subsequence of $\{\mathbf{w}_M\}_{M\in\mathbb{N}}$ converging weakly in $L^2(0,T;H^1(\Omega))$.

□

3.6. **Proof of the existence theorem.**

PROOF OF THEOREM 3.1. It remains to show that the triple $(\mathbf{c}, \mathbf{w}, \mathbf{u})$ obtained in the previous subsection is a weak solution in the sense of Definition 3.1. Therefore we need to pass to the limit in (3.15)-(3.17) using the convergence properties obtained above.

Equation (3.22) implies that for all $\boldsymbol{\xi} \in L^2(0,T;H^1(\Omega,\mathbb{R}^N))$ with $\partial_t\boldsymbol{\xi} \in L^2(\Omega_T)$ and $\boldsymbol{\xi}(T)=0$

$$-\int_{\Omega_T} \partial_t\boldsymbol{\xi}(\bar{\mathbf{c}}_M - \mathbf{c}^0) + \int_{\Omega_T} \mathbf{L}\nabla\mathbf{w}_M : \nabla\boldsymbol{\xi} = 0.$$

Using the convergence properties of $\bar{\mathbf{c}}_M$ and $\mathbf{w}_M$ (see Lemmas 3.4 and 3.5) we obtain the first equality (see (3.4)) in the definition of a weak solution.

Choosing a $\boldsymbol{\zeta} \in L^2(0,T;H^1(\Omega,\mathbb{R}^N)) \cap L^\infty(\Omega_T,\mathbb{R}^N)$ we conclude from (3.16)

$$\int_{\Omega_T} \mathbf{w}_M \cdot \boldsymbol{\zeta} = \int_{\Omega_T} \left\{ \boldsymbol{\Gamma}\nabla\mathbf{c}_M : \nabla\mathbf{P}\boldsymbol{\zeta} + \mathbf{P}\Psi_{,\mathbf{c}}(\mathbf{c}_M)\cdot\boldsymbol{\zeta} + \mathbf{P}W_{,\mathbf{c}}(\mathbf{c}_M, \nabla\mathcal{E}(\mathbf{u}_M))\cdot\boldsymbol{\zeta} \right\}.$$

Clearly the linear terms converge to the analogous expressions in (3.5). The convergence

$$\int_{\Omega_T} \Psi_{,\mathbf{c}}(\mathbf{c}_M)\cdot\boldsymbol{\zeta} \to \int_{\Omega_T} \Psi_{,\mathbf{c}}(\mathbf{c})\cdot\boldsymbol{\zeta}$$

follows with the help of the convergence theorem of Vitali by using the growth condition on $\Psi_{,\mathbf{c}}$ (see (A3.2)), the estimate on $\Psi^1(\mathbf{c}_M)$ in (3.21), the convergence almost everywhere of $\mathbf{c}_M$ and the boundedness of $\boldsymbol{\zeta}$. The generalised convergence theorem of Lebesgue, the growth assumption (A4.3) together with the strong convergence of $\nabla\mathbf{u}_M$ and $\mathbf{c}_M$ in L^2 yields that we can pass to the limit in $\int_{\Omega_T} W_{,\mathbf{c}}(\mathbf{c}_M, \mathcal{E}(\mathbf{u}_M))\cdot\boldsymbol{\zeta}$.

To pass to the limit in the elasticity system (3.17) is straightforward using again the strong convergence of $\nabla\mathbf{u}_M$ and $\mathbf{c}_M$ in $L^2(\Omega_T)$ and the growth condition (A4.3). $\square$

4. Uniqueness for homogeneous linear elasticity

We now prove a uniqueness theorem in the case of homogeneous linear elasticity and under the assumption that the stress free strain varies linearly with the concentration, i.e.

$$\mathcal{E}^\star(\mathbf{c}) = \sum_{k=1}^N c_k \mathcal{E}_k^\star, \tag{4.1}$$

where the $\mathcal{E}_k^\star = \mathcal{E}^\star(\mathbf{e}_k)$ are the stress free strains in the case that the material were uniformly equal to component k. Altogether the elastic part of the free energy has the form

$$W(\mathbf{c},\mathcal{E}) = \tfrac{1}{2}\left(\mathcal{E} - \mathcal{E}^\star(\mathbf{c})\right) : \mathcal{C}\left(\mathcal{E} - \mathcal{E}^\star(\mathbf{c})\right) \tag{4.2}$$

with a constant positive definite tensor $\mathcal{C}$ which is assumed to fulfil the usual symmetry conditions of linear elasticity (see [20]). Let us note explicitely that we do not assume that $\mathcal{C}$ is isotropic. This takes into account that in applications $\mathcal{C}$ in general will be an anisotropic tensor. Now the elastically modified Cahn-Hilliard system becomes

$$\begin{aligned} \partial_t \mathbf{c} &= \mathbf{L}\Delta \mathbf{w}, \\ \mathbf{w} &= \mathbf{P}\left(-\nabla\cdot\mathbf{\Gamma}\nabla\mathbf{c} + \Psi_{,\mathbf{c}}(\mathbf{c}) - \left(\mathcal{E}_k^\star : \mathcal{C}\left(\mathcal{E}(\mathbf{u}) - \mathcal{E}^*(\mathbf{c})\right)\right)_{k=1,\dots,N}\right), \\ 0 &= \nabla\cdot\mathcal{C}\left(\mathcal{E}(\mathbf{u}) - \mathcal{E}^\star(\mathbf{c})\right) \end{aligned} \tag{4.3}$$

which has to be solved together with the boundary conditions (2.11)-(2.13) and the initial condition (2.14).

Assume there exist two weak solutions $(\mathbf{c}_1, \mathbf{w}_1, \mathbf{u}_1)$ and $(\mathbf{c}_2, \mathbf{w}_2, \mathbf{u}_2)$, which solve the elastic Cahn-Hilliard system in the sense of Definition 3.1. Then formally it holds (compare Subsection 3.1)

$$\begin{aligned} &\tfrac{1}{2}\frac{d}{dt}\|\mathbf{c}_2 - \mathbf{c}_1\|_{\mathbf{L}}^2 + \int_\Omega \mathbf{\Gamma}\nabla(\mathbf{c}_2 - \mathbf{c}_1) : \nabla(\mathbf{c}_2 - \mathbf{c}_1) \\ &\quad + \int_\Omega \left(\Psi_{,\mathbf{c}}(\mathbf{c}_2) - \Psi_{,\mathbf{c}}(\mathbf{c}_1)\right)\cdot(\mathbf{c}_2 - \mathbf{c}_1) \\ &\quad + \int_\Omega \left(\mathcal{E}(\mathbf{u}_2 - \mathbf{u}_1) - \mathcal{E}^\star(\mathbf{c}_2 - \mathbf{c}_1)\right) : \mathcal{C}\left(\mathcal{E}(\mathbf{u}_2 - \mathbf{u}_1) - \mathcal{E}^\star(\mathbf{c}_2 - \mathbf{c}_1)\right) \\ &= 0. \end{aligned}$$

Our goal is to use this identity together with the convexity of Ψ^1, suitable conditions on Ψ^2 and the inequalities of Gronwall and Korn to prove uniqueness with respect to $\mathbf{c}$ and $\mathbf{u}$. Then the identity (2.8) gives uniqueness with respect to $\mathbf{w}$.

Theorem 4.1. *Assume (A1)-(A3) and (A5)-(A7), suppose $\Psi^2_{,\mathbf{c}}$ is globally Lipschitz continuous and let W have the form (4.1), (4.2).*

Then there exists a unique weak solution of the elastic Cahn-Hilliard system in the sense of Definition 3.1.

Proof. To prove the uniqueness result we generalise an idea of Blowey and Elliott [5] to the case that elastic effects are included. Assume there are two solutions $(\mathbf{c}_1, \mathbf{w}_1, \mathbf{u}_1)$ and $(\mathbf{c}_2, \mathbf{w}_2, \mathbf{u}_2)$ in the class $L^2(0,T;H^1(\Omega,\mathbb{R}^N)) \times L^2(0,T;H^1(\Omega,\mathbb{R}^N)) \times L^2(0,T;X_2)$. We define

$$\mathbf{c} := \mathbf{c}_2 - \mathbf{c}_1, \quad \mathbf{w} := \mathbf{w}_2 - \mathbf{w}_1, \quad \mathbf{u} = \mathbf{u}_2 - \mathbf{u}_1.$$

Then it holds

$$-\int_{\Omega_T} \mathbf{c}\cdot\partial_t\boldsymbol{\xi} + \int_{\Omega_T} \mathbf{L}\nabla\mathbf{w} : \nabla\boldsymbol{\xi} = 0$$

for all $\boldsymbol{\xi} \in L^2(0,T;H^1(\Omega,\mathbb{R}^N))$ with $\partial_t\boldsymbol{\xi} \in L^2(\Omega_T)$ and $\boldsymbol{\xi}(T) = 0$. For $t_0 \in (0,T)$ and given $\boldsymbol{\eta} \in L^2(0,T;H^1(\Omega,\mathbb{R}^N))$ we define

$$\boldsymbol{\xi}(.,t) := \begin{cases} \int_t^{t_0} \boldsymbol{\eta}(.,s)\,ds & \text{if } t \leq t_0, \\ 0 & \text{if } t > t_0. \end{cases}$$

Then we have

$$\begin{aligned} 0 &= \int_{\Omega_{t_0}} \mathbf{c}\cdot\boldsymbol{\eta} + \int_{\Omega_{t_0}} \mathbf{L}\nabla\mathbf{w} : \nabla\left(\int_t^{t_0} \boldsymbol{\eta}\right) \\ &= \int_{\Omega_{t_0}} \mathbf{c}\cdot\boldsymbol{\eta} + \int_{\Omega_{t_0}} \mathbf{L}\nabla\left(\int_0^t \mathbf{w}\right) : \nabla\boldsymbol{\eta}. \end{aligned} \tag{4.4}$$

This implies

$$\mathcal{G}\mathbf{c}(.,t) = -\int_0^t \mathbf{w}(.,s)ds \quad \text{and} \quad \partial_t\mathcal{G}\mathbf{c} = -\mathbf{w}.$$

Taking $\boldsymbol{\eta} = \mathbf{w}$ in (4.4) gives

$$0 = \int_{\Omega_{t_0}} \mathbf{c}\cdot\mathbf{w} + \int_{\Omega_{t_0}} \mathbf{L}\nabla\left(\mathcal{G}\mathbf{c}\right) : \nabla\left(\partial_t\mathcal{G}\mathbf{c}\right).$$

Since the second integrand is a time derivative, we can use $\mathbf{c}(0) = \mathcal{G}\mathbf{c}(0) = 0$ to obtain

$$0 = \int_{\Omega_{t_0}} \mathbf{c}\cdot\mathbf{w} + \int_{\Omega} \mathbf{L}\nabla(\mathcal{G}\mathbf{c}) : \nabla(\mathcal{G}\mathbf{c})(t_0). \tag{4.5}$$

Taking the difference of the equation (3.5) for $\mathbf{w}_2$ and $\mathbf{w}_1$ we obtain

$$\begin{aligned} \int_{\Omega_T} \mathbf{w}\cdot\boldsymbol{\zeta} &= \int_{\Omega_T} \Big\{\boldsymbol{\Gamma}\nabla\mathbf{c} : \nabla\boldsymbol{\zeta} + \left(\Psi_{,\mathbf{c}}(\mathbf{c}_2) - \Psi_{,\mathbf{c}}(\mathbf{c}_1)\right)\cdot\mathbf{P}\boldsymbol{\zeta} \\ &\qquad - \left(\mathcal{E}_k^\star : \mathcal{C}\left(\mathcal{E}(\mathbf{u}) - \mathcal{E}^*(\mathbf{c})\right)\right)_{k=1,\ldots,N}\cdot\mathbf{P}\boldsymbol{\zeta}\Big\} \end{aligned}$$

for all $\boldsymbol{\zeta} \in L^2(0,T;H^1(\Omega,\mathbb{R}^N)) \cap L^\infty(\Omega_T,\mathbb{R}^N)$. Now we choose the test function $\boldsymbol{\zeta} = \mathcal{X}_{[0,t_0]}\mathbf{P}_M(\mathbf{c}) = \mathcal{X}_{[0,t_0]}\mathbf{P}_M(\mathbf{c}_2 - \mathbf{c}_1)$, where we defined

$$\mathbf{P}_M(\mathbf{c}') := \begin{cases} \mathbf{c}' & \text{if } |\mathbf{c}'| \leq M, \\ \frac{\mathbf{c}'}{|\mathbf{c}'|}M & \text{if } |\mathbf{c}'| > M, \end{cases}$$

for all $M > 0$ and all $\mathbf{c}' \in \mathbb{R}^N$. Then the inequality

$$\left(\Psi^1_{,\mathbf{c}}(\mathbf{c}_2) - \Psi^1_{,\mathbf{c}}(\mathbf{c}_1)\right)\cdot\mathbf{P}_M\left(\mathbf{c}_2 - \mathbf{c}_1\right) \geq 0$$

leads to

$$\int_{\Omega_{t_0}} \Big\{ \boldsymbol{\Gamma}\nabla \mathbf{c} : \nabla \mathbf{P}_M(\mathbf{c}) + \left(\Psi^2_{,\mathbf{c}}(\mathbf{c}_2) - \Psi^2_{,\mathbf{c}}(\mathbf{c}_1)\right) \cdot \mathbf{P}_M\left(\mathbf{c}\right) \tag{4.6}$$
$$- \left(\mathcal{E}^\star_k : \mathcal{C}\left(\mathcal{E}(\mathbf{u}) - \mathcal{E}^*(\mathbf{c})\right)\right)_{k=1,\dots,N} \cdot \mathbf{P}_M\left(\mathbf{c}\right) - \mathbf{w} \cdot \mathbf{P}_M\left(\mathbf{c}\right) \Big\} \leq 0.$$

In the limit $M \to \infty$ we obtain (4.6) with $\mathbf{P}_M(\mathbf{c})$ replaced by $\mathbf{c}$.

Now we choose $\mathbf{u} = (\mathbf{u}_2 - \mathbf{u}_1)\mathcal{X}_{(0,t_0)}$ as a test function in the difference of the equations for $\mathbf{u}_2$ and $\mathbf{u}_1$ (see (4.3)), to discover

$$\int_{\Omega_{t_0}} \mathcal{C}\left(\mathcal{E}(\mathbf{u}) - \mathcal{E}^\star(\mathbf{c})\right) : \mathcal{E}(\mathbf{u}) = 0. \tag{4.7}$$

Using (4.5), (4.6) and (4.7) we obtain

$$\begin{aligned} \|\mathbf{c}\|_{\mathbf{L}}(t_0) \quad &+ \int_{\Omega_{t_0}} \boldsymbol{\Gamma}\nabla\mathbf{c} : \nabla\mathbf{c} + \int_{\Omega_{t_0}} \left(\mathcal{E}(\mathbf{u}) - \mathcal{E}^\star(\mathbf{c})\right) : \mathcal{C}\left(\mathcal{E}(\mathbf{u}) - \mathcal{E}^\star(\mathbf{c})\right) \\ &\leq \ - \int_{\Omega_{t_0}} \left(\Psi^2_{,\mathbf{c}}(\mathbf{c}_2) - \Psi^2_{,\mathbf{c}}(\mathbf{c}_1)\right) \cdot \mathbf{c}. \end{aligned}$$

Taking into account the Lipschitz continuity of $\Psi^2_{,\mathbf{c}}$ we can use (3.1) and the Gronwall inequality to conclude

$$\|\mathbf{c}\|_{\mathbf{L}} = 0 \quad \text{ and hence } \mathbf{c} = 0.$$

Then we obtain

$$\int_{\Omega_T} \mathcal{E}(\mathbf{u}) : \mathcal{C}\mathcal{E}(\mathbf{u}) = 0$$

and Korn's inequality (see Theorem 5.2) implies

$$\mathbf{u} = 0.$$

Now (3.5) ensures that $\mathbf{w}$ is uniquely defined. This completes the proof of the uniqueness theorem. □

5. Appendix

In this section we collect some known results used in the text.

Theorem 5.1. (Generalised Lebesgue convergence theorem) *Assume $E \subset \mathbb{R}^n$ is measurable, $g_n \longrightarrow g$ in $L^q(E)$ with $1 \leq q < \infty$ and $f_n, f : E \longrightarrow \mathbb{R}^n$ are measurable functions such that*

$$\begin{aligned} f_n &\longrightarrow f \qquad && a.e. \ in \ \ E\,, \\ |f_n|^p &\leq |g_n|^q && a.e. \ in \ E \end{aligned}$$

with $1 \leq p < \infty$. Then $f_n \longrightarrow f$ in $L^p(E)$.

For a proof see [1].

Theorem 5.2. (Korn's inequality) *Let Ω be a bounded domain with Lipschitz boundary.*
There exists a constant $c > 0$ such that

$$\int_\Omega \mathcal{E}(\mathbf{u}) : \mathcal{E}(\mathbf{u}) \geq c\|\mathbf{u}\|^2_{H^1}$$

for all $u \in X_2 := \{\mathbf{u} \in H^1(\Omega, \mathbb{R}^n) \,|\, (\mathbf{u}, \mathbf{v})_{H^1} = 0$ for all $\mathbf{v} \in X_{ird}\} = X_{ird}^{\perp}$ where $X_{ird} := \{\mathbf{u} \in H^1(\Omega, \mathbb{R}^n) \,|\,$ there exist $\mathbf{b} \in \mathbb{R}^n$ and a skew symmetric $\mathbf{A} \in \mathbb{R}^{n\times n}$ such that $\mathbf{u}(\mathbf{x}) = \mathbf{b} + \mathbf{A}\mathbf{x}\}$.

A proof can be found for example in Zeidler [47].

Theorem 5.3. (Arzelà-Ascoli theorem) *Let B be a Banach space. A subset F of $C([0,T]; B)$ is relatively compact if and only if:*
(i) $\{f(t) \,|\, f \in F\}$ is relatively compact in B for all $t \in (0,T)$,
(ii) F is uniformly equicontinuous, i.e. for all $\varepsilon > 0$ there exists a $\delta > 0$ such that

$$\|f(t_2) - f(t_1)\|_B \leq \varepsilon$$

for all $f \in F$, and $t_1, t_2 \in [0,T]$ such that $|t_2 - t_1| \leq \delta$.

For a proof we refer to Simon [43].

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Harald Garcke,
NWF I - Mathematik,
93040 Regensburg, Germany,
harald.garcke@mathematik.uni-regensburg.de