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NUMERICAL APPROXIMATION OF THE CAHN-LARCHÉ EQUATION

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Abstract. Spinodal decomposition, i.e., the separation of a homogeneous mixture into different phases, can be modeled by the Cahn-Hilliard equation - a fourth order semilinear parabolic equation. If elastic stresses due to a lattice misfit become important, the Cahn-Hilliard equation has to be coupled to an elasticity system to take this into account. Here, we present a discretization based on finite elements and an implicit Euler scheme. We first show solvability and uniqueness of solutions. Based on an energy decay property we then prove convergence of the scheme. Finally we present numerical experiments showing the impact of elasticity on the morphology of the microstructure.

Key words and phrases. Cahn-Hilliard equation, Cahn-Larché equation, fourth order parabolic equation, elasticity, finite element approximation,second order time discretization

Mathematics Subject classification. 35K35, 35K55, 65L50, 65M12, 65M15, 65M60, 82B26

1. Introduction

The kinetics of phase separation in a binary alloy after quenching is characterized by three stages. Since for low temperatures the initially homogeneous state is unstable, first, domains of a new phase nucleate and grow rapidly in a second stage. Then, two phases have formed and are separated by interfacial layers which are much thinner than the typical diameter of the domains. In the last stage of the phase separation the system is driven by the reduction of the surface energy of these interfacial layers, which leads to an increase of the typical length scales in the system, a phenomenon known as coarsening.

In the case of negligible elastic effects, particles tend to become round and phase separation is well-described by the Cahn-Hilliard equation. 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 spacings of the alloy components. The inclusion of elastic effects into the Cahn-Hilliard model yields the Cahn-Larché model.

In Figure 1 we demonstrate the effects that anisotropic elastic energy and different lattice spacings 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 [10]). Furthermore numerical simulations indicate this.

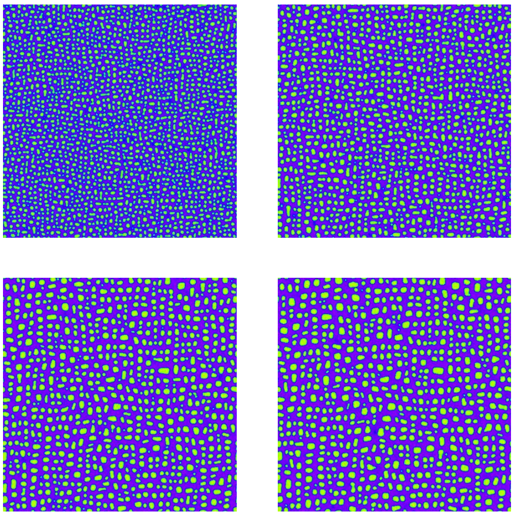


Figure 1. Evolution with inhomogeneous, anisotropic elasticity

After stating both the Cahn-Hilliard- and the Cahn-Larché model we present a discretization based on finite elements and an implicit Euler scheme. The main part of the paper is devoted to the analysis of this numerical scheme. We first show solvability and uniqueness of solutions to the discrete scheme. Based on an energy decay property we then prove convergence of the scheme. The proof uses ideas of the proof of existence of solutions for the continuous problem in [11]. In [12] we have analysed a corresponding discretization for the case of homogeneous elasticity, i.e. where the elasticity tensor does not depend on the concentration. The paper [12] also contains error estimates for homogeneous elasticity. For inhomogeneous elasticity no uniqueness result is known and therefore it does not seem possible to show error estimates before the uniqueness question has been answered. In the final section of this paper we present numerical results highlighting the additional qualitative effects of the elastic interactions.

Finally, we remark that many authors used spectral methods to solve the Cahn-Larché system. We refer e.g. to the work by Dreyer and Müller [5] and by Leo, Lowengrub and Jou [18] and the references therein. Due to the highly nonlinear structure of the Cahn-Larché system, approaches based on spectral methods loose their efficiency. This is in particular true in the case that the elastic constants are different in the two phases (inhomogeneous ealsticity). We also remark that to our knowledge this is the first paper on the numerical analysis of the Cahn-Larché system in the case of inhomogeneous elasticity.

2. The continuous model

The Cahn-Hilliard equation. The Cahn–Hilliard model has been proposed in [2]. It describes the evolution of the relative concentration difference $\rho = (2\frac{\rho_A}{\rho_A+\rho_B} - 1)$, where ρ_A and ρ_B are the concentrations of the two components.

The corresponding Ginzburg–Landau free energy E is defined to be

$$E_{C.H.}(\rho) := \int\limits_{\Omega} \left\{ \psi(\rho) + \frac{\gamma}{2}|\nabla \rho|^2 \right\} dx, \tag{2.1}$$

where Ω is a bounded domain in $\mathbb{R}^d$ $(d = 1, 2, 3)$ and γ a positive parameter. The first term in the free energy, $\psi(\rho)$, is the chemical free energy density and typically has a double well form. In this paper we take

$$\psi(\rho) = \frac{1}{4}\left(\rho^2 - 1\right)^2. \tag{2.2}$$

We note that the system is locally in one of the two phases if the value of ρ is close to one of the two minima ± 1 of ψ. The second term in the energy penalizes gradients with the effect that the total amount of transition zones is accounted for in the energy.

Now, the diffusion equation for the concentration ρ is given by

$$\frac{\partial \rho}{\partial t} = \Delta w \tag{2.3}$$

on $\Omega \times \mathbb{R}^+$. In the equation above we denote by w the local chemical potential difference which is given as the variational derivative $\frac{\delta E_{C.H.}}{\delta \rho}$ of $E_{C.H.}$ with respect to ρ. Thus, we obtain

$$w = \psi'(\rho) - \gamma \Delta \rho. \tag{2.4}$$

The system has to be supplemented with boundary and initial conditions. Here we prescribe $\partial_\nu w = \partial_\nu \rho = 0$, where ν is the outer normal on $\partial\Omega$, and $\rho(\cdot, 0) = \rho_0(\cdot)$ for some initial concentration distribution ρ_0. Roughly speaking the model describes diffusion of the species in such a way that the energy functional (2.1) is minimized as quickly as possible under a mass preserving constraint. For surveys regarding the modelling and the corresponding analysis see [6, 20, 10]. Gurtin proposes in [13] an alternative approach yielding the same system of equations. Existence of solutions has been shown in [8].

The Cahn-Larché model. In order to include elastic effects we consider the displacement field $\mathbf{u}$ as an additional quantity. The Ginzburg–Landau free energy E in the extended Cahn-Larché model is defined to be

$$E(\rho, \mathbf{u}) := \int_{\Omega} \left\{ \psi(\rho) + \frac{\gamma}{2}|\nabla \rho|^2 + W(\rho, \mathcal{E}(\mathbf{u})) \right\} dx.$$

Now the free energy consists of three terms where the third term accounts for energy contributions due to elastic effects. Since the deformations that appear in applications are usually small, the theory is based on linear elasticity and therefore the strain tensor is given by

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

In the case of homogeneous elasticity, i.e. in the case that the elastic constants in the two phases are the same, the elastic energy is (see e.g. [9, 10, 16])

$$W(\rho,\mathcal{E}) = \left(\mathcal{E} - \bar{\mathcal{E}}(\rho)\right) : \mathcal{C}\left(\mathcal{E} - \bar{\mathcal{E}}(\rho)\right). \tag{2.5}$$

Here, $\mathcal{C}$ is the possibly anisotropic elasticity tensor which we assume to be positive definite and complying with the usual symmetry conditions of linear elasticity:

$$\mathcal{C}_{ijmn} = \mathcal{C}_{ijnm} = \mathcal{C}_{jimn}\ , \qquad\qquad \mathcal{C}_{ijmn} = \mathcal{C}_{mnij}.$$

The term $\bar{\mathcal{E}}(\rho)$ is the stress free strain at a concentration ρ. This is the value the strain tensor would take if the material is uniform with concentration ρ. We will assume that Vegard's law is satisfied, i.e. the stress free strain is isotropic and varies linearly with the concentration. Hence (see [10]),

$$\bar{\mathcal{E}}(\rho) = e(\rho - \bar{\rho})\mathbb{1}$$

with constants e, $\bar{\rho}$ and the identity matrix $\mathbb{1}$. In the following we will take without loss of generality $\bar{\rho} = 0$ which means that we take a reference state that is a uniform mixture of the two components. The product $A : B$ of two $d \times d$ matrices A, B is defined to be the $\sum_{i,j=1}^{d} A_{ij}B_{ij}$.

The case of inhomogeneous elasticity is more complicated but shows richer effects. We consider the following structure

$$\mathcal{C}(\rho) = \mathcal{C}^P + m(\rho)(\mathcal{C}^M - \mathcal{C}^P)$$

with constant tensors $\mathcal{C}^P$, $\mathcal{C}^M$ and a smooth interpolation function $m(.)$ with the property

$$m(-1) = 0\ , \qquad m(1) = 1\,, \\ m'(-1) = 0\ , \qquad m'(1) = 0.$$

In particular we choose

$$m(t) = \begin{cases} 0 & \text{for } t \le -1\,, \\ \frac{1}{4}\left(-t^3 + 3t + 2\right) & \text{for } -1 < t < 1\,, \\ 1 & \text{for } 1 \le t. \end{cases}$$

For the constant tensors $\mathcal{C}^P$ and $\mathcal{C}^M$ we assume positive definiteness and the above mentioned symmetry conditons.

The diffusion equation for the concentration ρ is again given by (2.3). And the chemical potential difference w is also given as the variational derivative $\frac{\delta E}{\delta \rho}$ of E with respect to ρ. With the additional elastic contribution in the energy we obtain $w = -\gamma\Delta\rho + \psi'(\rho) + W_{,\rho}(\rho, \mathcal{E}(\mathbf{u}))$ with

$$W_{,\rho}(\rho,\mathcal{E}(\mathbf{u})) = -e\mathbb{1} : \mathcal{C}(\rho)\left(\mathcal{E}(\mathbf{u}) - \bar{\mathcal{E}}(\rho)\right) + \frac{1}{2}\left(\mathcal{E}(\mathbf{u}) - \bar{\mathcal{E}}(\rho)\right) : \mathcal{C}'(\rho)\left(\mathcal{E}(\mathbf{u}) - \bar{\mathcal{E}}(\rho)\right).$$

Since the relaxation into mechanical equilibrium occurs on a time scale that is fast compared to the time scale at which diffusion takes place we assume quasistatic equilibrium for the deformation. Hence, $\frac{\delta E}{\delta \mathbf{u}} = 0$ which implies $\operatorname{div} \mathcal{S} = 0$ where

$$\mathcal{S} = \mathcal{C}(\rho)(\mathcal{E}(\mathbf{u}) - \bar{\mathcal{E}}(\rho))$$

is the stress tensor. We confine ourselves to stress free boundary conditions, i.e. $\mathcal{S}\nu = 0$.

Summing up the system comprises the following two equations for ρ and $\mathbf{u}$ on $\Omega \times [0, T]$:

$$\begin{aligned} \partial_t \rho &= \Delta \Big[\psi'(\rho) - \gamma \Delta \rho - e\mathbb{1} : \mathcal{C}(\rho) \big(\mathcal{E}(\mathbf{u}) - \bar{\mathcal{E}}(\rho) \big) \\ &\qquad + \frac{1}{2} \big(\mathcal{E}(\mathbf{u}) - \bar{\mathcal{E}}(\rho) \big) : \mathcal{C}'(\rho) \big(\mathcal{E}(\mathbf{u}) - \bar{\mathcal{E}}(\rho) \big) \Big], \end{aligned} \tag{2.6}$$

$$0 = \operatorname{div} \big(\mathcal{C}(\rho)(\mathcal{E}(\mathbf{u}) - \bar{\mathcal{E}}(\rho)) \big). \tag{2.7}$$

One can easily verify that solutions of the system (2.6), (2.7) with the above specified boundary conditions fulfill

$$\frac{d}{dt} \int\limits_{\Omega} \rho = 0 \quad \text{and} \quad \frac{d}{dt} E(\rho, u) \leq 0.$$

These properties will be important ingredients in our convergence analysis. The modelling of the elastic material properties as presented here is due to Khachaturyan [15]. In [17] Cahn and Larché considered this system for the case $\gamma = 0$ and for $\gamma > 0$ it was studied by Onuki [21].

3. THE DISCRETIZATION

We want to solve (2.6)-(2.7) on the set $\Omega_T := \Omega \times (0, T)$ where $T > 0$ is a fixed time. Therefore, we subdivide the time intervall $[0, T]$ into N steps with length τ_n and set $t_n := \sum_{i=1}^{n} \tau_i$. In addition let $t_0 = 0$ and $\tau = \max_{n=1,\dots,N} \{\tau_n\}$.

In the following we will assume for simplicity that Ω is a polyhedral domain. Generalisations to curved domains are of course possible by using boundary finite elements with curved faces (see e.g. Ciarlet [3]). We construct triangulations $\mathcal{T}^h$ – which we suppose to be regular in the sense of [3] – with maximal element size $h := \max_{s \in \mathcal{T}^h} \{\operatorname{diam} s\}$.

Associated to $\mathcal{T}^h$ is a finite element space of continuous piecewise affine elements

$$V^h := \Big\{ \varphi \in C^0(\bar{\Omega}) \Big| \varphi\big|_T \in P_1(T) \ \forall T \in \mathcal{T}^h \Big\} \subset H^{1,2}(\Omega).$$

Here, we denoted by $P_1(T)$ the set of all affine linear functions on T.

To write the elastic terms more conveniently we introduce the following scalar product of two matrix-valued functions $\mathcal{A}$ and $\mathcal{B}$:

$$\langle \mathcal{A}, \mathcal{B} \rangle_{\mathcal{C}(\rho)} := \int\limits_{\Omega} \mathcal{A} : \mathcal{C}(\rho) \mathcal{B} \, dx.$$

Furthermore, we use the lumped mass scalar product $(.,.)^h$ instead of the L^2-scalar product $(.,.)$ where appropriate and make use of the following approximating properties (see [7]): For $v \in C^0(\bar{\Omega})$ let $|v|_h := \sqrt{(v,v)^h}$, then there are constants c_0 and c_1 such that for any $\varphi^h \in V^h$

$$c_0 \left\|\varphi^h\right\|_{L^2(\Omega)} \leq \left|\varphi^h\right|_h \leq c_1 \left\|\varphi^h\right\|_{L^2(\Omega)} . \tag{3.1}$$

The implicit Euler scheme. The numerical analysis below is based on the following scheme:

For $n = 1, \ldots, N$ and given $\rho^h_{n-1} \in V^h$ find $\rho^h_n \in V^h, \mathbf{u}^h_n \in (V^h)^d$, $w^h_n \in V^h$ such that for any $\varphi^h \in V^h$ and any $\boldsymbol{\xi}^h \in (V^h)^d$:

$$\left(\frac{\rho^h_n - \rho^h_{n-1}}{\tau_n}, \varphi^h\right)^h = -\left(\nabla w^h_n, \nabla\varphi^h\right), \tag{3.2}$$

$$\left(w^h_n, \varphi^h\right)^h = \left(\psi'(\rho^h_n), \varphi^h\right)^h + \gamma\Big(\nabla\rho^h_n, \nabla\varphi^h\Big) + \left(W_{,\rho}(\rho^h_n, \mathcal{E}(\mathbf{u}^h_n)), \varphi^h\right), \tag{3.3}$$

$$0 = \left\langle \mathcal{E}(\mathbf{u}^h_n) - \bar{\mathcal{E}}(\rho^h_n), \mathcal{E}(\boldsymbol{\xi}^h)\right\rangle_{\mathcal{C}(\rho^h_n)} . \tag{3.4}$$

The solution $\mathbf{u}^h_n$ is not unique. We can add any function that lies in the kernel of the operator $\mathcal{E}$, i.e. we can add any infinitesimal rigid motion (see [14]). We always choose the unique solution that has minimal L^2-norm under all solutions. This makes it possible to apply Korn's inequality and does not change the evolution law for ρ^h_n (the quantity we are interested in) as only $\mathcal{E}(\mathbf{u}^h_n)$ enters the equation for ρ^h_n. The first summand of the right hand side of (3.3) involve the integration of functions that are not piecewise affine. Hence, the lumped mass scalar product gives not exactly the same results as the L^2-scalar product here.

Analysis of the discrete scheme

In this section we show existence, uniqueness and boundedness of solutions of the discrete scheme and identify its solution as the global minimizer of an energy functional E^n. We proceed as follows: After establishing existence of minimizers of E^n we identify the scheme (3.2)–(3.4) with the Euler-Lagrange equations of E^n. This implies solvability of (3.2)–(3.4). If τ_n is not too large we can derive bounds on the solution that allow us to prove uniqueness of the solution of the discrete scheme. It then follows that a solution to (3.2)–(3.4) is in fact the global minimizer of E^n.

Solvability. We consider in each timestep the functional on $V^h \times (V^h)^d$:

$$E^n(r,\mathbf{v}) := \int_\Omega \left\{\frac{1}{2\tau_n}\left|\nabla\Delta_h^{-1}(r-\rho^h_{n-1})\right|^2 + \frac{\gamma}{2}|\nabla r| + W(r,\mathcal{E}(\mathbf{v}))\right\} dx + \Big(\psi(r),1\Big)^h,$$

where the operator $\Delta_h^{-1} : V^h \longrightarrow V^h$ is defined via: For a given function $f^h \in V^h$ with $\int_\Omega f^h = 0$, let $v^h = \Delta_h^{-1} f^h$ be the solution of

$$\left(f^h, \varphi^h\right)^h = -\left(\nabla v^h, \nabla \varphi^h\right) \qquad\qquad \forall \varphi^h \in V^h,$$

that fulfills $\int_\Omega v^h \, dx = 0$.

As E^n is bounded from below and continuous on the finite dimensional space $V^h \times (V^h)^d$ the existence of a global minimizer $(\bar{\rho}^h,\ \bar{\mathbf{u}}^h)$ follows immediately using the fact that E^n is coercive when we restrict ourselves to all $\mathbf{u}^h$ that are perpendicular in L^2 to the kernel of $\mathcal{E}$. Here we use Korn's inequality (see e.g. Zeidler [23]). Via the direct method of the calculus of variation one can even show that the extension of E^n to $H^{1,2} \times (H^{1,2})^d$ has minimizers for sufficiently small τ_n (see [11]).

The Euler-Lagrange equations of E^n. The first variation of E^n in $(r, \mathbf{v})$ in the direction $(\varphi^h, \boldsymbol{\xi}^h)$ is

$$\begin{aligned}\delta E^n(r, \mathbf{v}; \varphi^h, \boldsymbol{\xi}^h) = {}& \frac{1}{\tau_n}\left(\nabla \Delta_h^{-1}(r - \rho_{n-1}^h), \nabla \Delta_h^{-1} \varphi^h\right) + \gamma\left(\nabla r, \nabla \varphi^h\right) \\ & + \left(\psi'(r), \varphi^h\right)^h + \left(W_{,\rho}(r, \mathcal{E}(\mathbf{v})), \varphi^h\right) + \left\langle \mathcal{E}(\mathbf{v}) - \bar{\mathcal{E}}(r), \mathcal{E}(\boldsymbol{\xi}^h)\right\rangle_{\mathcal{C}(r)}.\end{aligned}$$

As minimizers $\bar{\rho}^h, \bar{\mathbf{u}}^h$ solve the Euler-Lagrange equations

$$\begin{aligned}0 &= \delta E^n(\bar{\rho}^h, \bar{\mathbf{u}}^h; \varphi^h, \boldsymbol{\xi}^h) \\ &= \frac{1}{\tau_n}\left(\nabla \Delta_h^{-1}(\bar{\rho}^h - \rho_{n-1}^h), \nabla \Delta_h^{-1} \varphi^h\right) + \gamma\left(\nabla \bar{\rho}^h, \nabla \varphi^h\right) + \left(\psi'(\bar{\rho}^h), \varphi^h\right)^h \\ &\quad + \left(W_{,\rho}(\bar{\rho}, \mathcal{E}(\bar{\mathbf{u}}^h)), \varphi^h\right) + \left\langle \mathcal{E}(\bar{\mathbf{u}}^h) - \bar{\mathcal{E}}(\bar{\rho}^h), \mathcal{E}(\boldsymbol{\xi}^h)\right\rangle_{\mathcal{C}(\bar{\rho}^h)}\end{aligned}$$

for arbitrary $\varphi^h \in V_n^h$ and $\boldsymbol{\xi}^h \in (V_n^h)^d$. Definining $w_n^h := \Delta_h^{-1} \frac{\bar{\rho}^h - \rho_{n-1}^h}{\tau_n} + (\psi'(\bar{\rho}^h), 1)^h + (W_{,\rho}(\bar{\rho}^h, \mathcal{E}(\bar{\mathbf{u}}^h)), 1)$ we have from the definition of Δ_h^{-1}:

$$\left(\frac{\bar{\rho}^h - \rho_{n-1}^h}{\tau_n}, \varphi^h\right)^h = -\left(\nabla w_n^h, \nabla \varphi^h\right),$$

for any $\varphi^h \in V_n^h$, which is the first equation of the scheme (3.2)–(3.4). Choosing $\boldsymbol{\xi}^h = 0$ yields

$$\left(w_n^h, \varphi^h\right) = \gamma\left(\nabla \bar{\rho}^h, \nabla \varphi^h\right) + \left(\psi'(\bar{\rho}^h), \varphi^h\right)^h + \left(W_{,\rho}(\bar{\rho}^h, \mathcal{E}(\bar{\mathbf{u}}^h))\varphi^h\right)$$

and setting $\varphi^h = 0$ result in

$$0 = \left\langle \mathcal{E}(\bar{\mathbf{u}}^h) - \bar{\mathcal{E}}(\bar{\rho}^h), \mathcal{E}(\boldsymbol{\xi}^h)\right\rangle_{\mathcal{C}(\bar{\rho}^h)}.$$

Summing up we see that the Euler-Lagrange equations of E^n are indeed identical to the scheme (3.2)–(3.4) and the existence of minimizers of E^n then implies the solvability of (3.2)–(3.4).

Boundedness. In this section we show that if the time-steps are small enough general solutions of the discrete scheme are bounded in $H^{1,2}$ and by inverse inequalities also in L^∞ (for the last property we need a uniform triangulation). This is in order to show uniqueness to (3.2)–(3.4) if the time-step is not too large. We remark that the minimizer to E^n fulfills better a priori estimates then the one obtained in this section. But in general we cannot guarantee that we compute the absolute minimizer in practice.

Lemma (Boundedness of discrete solutions). *Let $\rho_n^h, w_n^h, \mathbf{u}_n^h$ be solutions of the discrete scheme. Then there are constants c_i $(i = 1, 2, 3)$ depending on ρ_{n-1}^h, γ, Ω, $\mathcal{C}^P$ and $\mathcal{C}^M$ such that for $\tau_n < c_1$ it holds*

$$\left\|\mathcal{E}(\mathbf{u}_n^h)\right\|_{L^2(\Omega)} < c_2\,,$$
$$\left\|\rho_n^h\right\|_{H^{1,2}(\Omega)} < c_3.$$

Proof. Choosing $\varphi^h = \tau_n w_n^h$ in (3.2) and $\varphi^h = -\rho_n^h$ in (3.3) gives

$$\begin{aligned}(3.5)\qquad \tau_n \left\|\nabla w_n^h\right\|_{L^2(\Omega)}^2 + \gamma \left\|\nabla \rho_n^h\right\|_{L^2(\Omega)}^2 + \left((\rho_n^h)^4, 1\right)^h \le \\ \left|\left(\rho_{n-1}^h, w_n^h - \frac{1}{|\Omega|}\int_\Omega w_n^h\right)^h\right| + \left|\int_\Omega \rho_{n-1}^h\right|\left|\frac{1}{|\Omega|}\int_\Omega w_n^h\right| + \\ \left((\rho_n^h)^2, 1\right)^h + c\left(\|\rho_n^h\|_{L^2(\Omega)}^2 + \left\|\mathcal{E}(\mathbf{u}_n^h) - \bar{\mathcal{E}}(\rho_n^h)\right\|_{L^2(\Omega)}^2\right).\end{aligned}$$

This holds because $\mathcal{C}'(\rho_n^h)\rho_n^h$ is bounded, which follows from the fact that $\mathcal{C}' = 0$ if $\left|\rho_n^h\right| > 1$.

Now we choose $\boldsymbol{\xi}^h = \mathbf{u}_n^h$ in (3.4) and obtain

$$(3.6)\qquad \left\|\mathcal{E}(\mathbf{u}_n^h)\right\|_{L^2(\Omega)}^2 \le c\left\|\rho_n^h\right\|_{L^2(\Omega)}^2.$$

Taking $\varphi^h = 1$ in (3.2) gives $\int_\Omega \rho_{n-1}^h = \int_\Omega \rho_n^h$ while the choice $\varphi^h = 1$ in (3.3) yields

$$\begin{aligned}(3.7)\qquad \left|\int_\Omega w_n^h\right| &\le \left|\left((\rho_n^h)^3 - \rho_n^h, 1\right)^h\right| + \left|(\rho_n^h, 1)\right| + \left|\int_\Omega W_{,\rho}(\rho_n^h, \mathcal{E}(\mathbf{u}_n^h))\right| \\ &\le c\left(\left|\left((\rho_n^h)^3, 1\right)^h\right| + \left\|\mathcal{E}(\mathbf{u}_n^h) - \bar{\mathcal{E}}(\rho_n^h)\right\|_{L^2(\Omega)}^2 + 1\right).\end{aligned}$$

Combining (3.5)-(3.7) and using Poincaré's and Young's inequality we get

$$\tau_n \left\|\nabla w_n^h\right\|_{L^2(\Omega)}^2 + \gamma \left\|\nabla \rho_n^h\right\|_{L^2(\Omega)}^2 + \left((\rho_n^h)^4, 1\right)^h \le \overline{C}\left(\left\|\rho_{n-1}^h\right\|_{L^2(\Omega)}^2 + \left\|\rho_n^h\right\|_{L^2(\Omega)}^2 + 1\right)$$

since the cubic term in (3.7) can be bounded by the quartic term in (3.5).

Taking $\varphi^h = \tau_n(\rho_n^h - \rho_{n-1}^h)$ in (3.2), using (3.1) and Young's inequality we obtain

$$\left\|\rho_n^h - \rho_{n-1}^h\right\|_{L^2(\Omega)}^2 \le \delta\left\|\nabla(\rho_n^h - \rho_{n-1}^h)\right\|_{L^2(\Omega)}^2 + {\tau_n}^2 \frac{C_\delta}{\delta}\left\|\nabla w_n^h\right\|_{L^2(\Omega)}^2.$$

Choosing δ such that $4\overline{C}\ \delta < \frac{\gamma}{2}$ we obtain

$$\left(\tau_n - {\tau_n}^2 \frac{2\overline{C}C_\delta}{\delta}\right) \left\|\nabla w_n^h\right\|_{L^2(\Omega)}^2 + \frac{\gamma}{2} \left\|\nabla \rho_n^h\right\|_{L^2(\Omega)}^2 \leq C(\rho_{n-1}^h, \gamma).$$

If $\tau_n < \frac{\delta}{2\overline{C}C_\delta}$ we have (again using Poincaré's inequality) a bound on $\left\|\rho_n^h\right\|_{H^{1,2}(\Omega)}$ and because of (3.6) also a bound on $\mathcal{E}(\mathbf{u}_n^h)$ in the $L^2(\Omega)$-Norm. ☐

Uniqueness. In this section we assume that the triangulations are uniform in order to make use of inverse inequalities (see [3]).

Lemma. Let $\{\mathcal{T}^h\}_{h>0}$ *be a family of uniform triangulations. The there exists a constant* $C_u > 0$ *depending on* $\|\rho_{n-1}^h\|_{H^1(\Omega)}$ *such that the solution of the scheme (3.2)–(3.4) is unique if* $\tau_n < C_u h^d$.

Proof. Given a fixed ρ_{n-1}^h let $\rho_a^h, w_a^h, \mathbf{u}_a^h$ and $\rho_b^h, w_b^h, \mathbf{u}_b^h$ be two solutions of the scheme (3.2)–(3.4). From the previous section we have, using an inverse inequality,

$$\left\|\rho_a^h\right\|_{L^\infty(\Omega)}, \left\|\rho_b^h\right\|_{L^\infty(\Omega)}, \left\|\mathcal{E}(\mathbf{u}_a^h)\right\|_{L^\infty(\Omega)}, \left\|\mathcal{E}(\mathbf{u}_b^h)\right\|_{L^\infty(\Omega)} < \frac{c}{h^{\frac{d}{2}}}.$$

Uniqueness of the elasticity system. We now show that $\left\|\mathcal{E}(\mathbf{u}_a^h) - \mathcal{E}(\mathbf{u}_b^h)\right\|_{L^2(\Omega)} \leq \frac{c}{h^{\frac{d}{2}}} \left\|\rho_a^h - \rho_b^h\right\|_{L^2(\Omega)}$. To see this let $\mathbf{u}_*^h$ be solution of

$$\left\langle \mathcal{E}(\mathbf{u}_*^h), \mathcal{E}(\boldsymbol{\xi}^h)\right\rangle_{\mathcal{C}(\rho_a^h)} = \left\langle \bar{\mathcal{E}}(\rho_b^h), \mathcal{E}(\boldsymbol{\xi}^h)\right\rangle_{\mathcal{C}(\rho_b^h)} \tag{3.8}$$

for all $\boldsymbol{\xi}^h \in (V^h)^d$. Combining this with (3.4) for $\mathbf{u}_a^h, \rho_a^h$ yields

$$\left\langle \mathcal{E}(\mathbf{u}_a^h) - \mathcal{E}(\mathbf{u}_*^h), \mathcal{E}(\boldsymbol{\xi}^h)\right\rangle_{\mathcal{C}(\rho_a^h)} = \left(\mathcal{E}(\boldsymbol{\xi}^h) : \left(\mathcal{C}(\rho_a^h)\bar{\mathcal{E}}(\rho_a^h) - \mathcal{C}(\rho_b^h)\bar{\mathcal{E}}(\rho_b^h)\right), 1\right).$$

Choosing $\boldsymbol{\xi}^h = \mathbf{u}_a^h - \mathbf{u}_*^h$ we gather using the smoothness of the interpolation function m

$$\left\|\mathcal{E}(\mathbf{u}_a^h) - \mathcal{E}(\mathbf{u}_*^h)\right\|_{L^2(\Omega)} \leq c \left\|\mathcal{C}(\rho_a^h)\bar{\mathcal{E}}(\rho_a^h) - \mathcal{C}(\rho_b^h)\bar{\mathcal{E}}(\rho_b^h)\right\|_{L^2(\Omega)} \leq c \left\|\rho_a^h - \rho_b^h\right\|_{L^2(\Omega)}. \tag{3.9}$$

Combining (3.8) with (3.4) for $\mathbf{u}_b^h, \rho_b^h$ we get

$$\left(\mathcal{E}(\boldsymbol{\xi}^h) : \left(\mathcal{C}(\rho_b^h)\mathcal{E}(\mathbf{u}_b^h) - \mathcal{C}(\rho_a^h)\mathcal{E}(\mathbf{u}_*^h)\right), 1\right) = 0$$

which is equivalent to

$$\left\langle \mathcal{E}(\mathbf{u}_*^h) - \mathcal{E}(\mathbf{u}_b^h), \mathcal{E}(\boldsymbol{\xi}^h)\right\rangle_{\mathcal{C}(\rho_a^h)} = \left(\mathcal{E}(\boldsymbol{\xi}^h) : \left(\left(\mathcal{C}(\rho_b^h) - \mathcal{C}(\rho_a^h)\right)\mathcal{E}(\mathbf{u}_b^h)\right), 1\right).$$

The choice $\boldsymbol{\xi}^h = \mathbf{u}_*^h - \mathbf{u}_b^h$ leads to

$$\left\|\mathcal{E}(\mathbf{u}_*^h) - \mathcal{E}(\mathbf{u}_b^h)\right\|_{L^2(\Omega)} \leq c \left\|\left(\mathcal{C}(\rho_b^h) - \mathcal{C}(\rho_a^h)\right)\mathcal{E}(\mathbf{u}_b^h)\right\|_{L^2(\Omega)} \leq \frac{c}{h^{\frac{d}{2}}} \left\|\rho_a^h - \rho_b^h\right\|_{L^2(\Omega)} \tag{3.10}$$

using the L^∞-bound on $\mathcal{E}(\mathbf{u}_b^h)$ and again the smoothness of m. The estimates (3.9) and (3.10) together imply

$$\left\|\mathcal{E}(\mathbf{u}_a^h)-\mathcal{E}(\mathbf{u}_b^h)\right\|_{L^2(\Omega)} \le \frac{c}{h^{\frac{d}{2}}}\left\|\rho_a^h-\rho_b^h\right\|_{L^2(\Omega)}. \tag{3.11}$$

Lipschitz continuity of $W_{,\rho}$. Let $F(\rho,\mathcal{E}) = e\mathbb{1} : \mathcal{C}(\rho)\big(\mathcal{E}-\bar{\mathcal{E}}(\rho)\big)$ and $G(\rho,\mathcal{E}) = \big(\mathcal{E}-\bar{\mathcal{E}}(\rho)\big) : \mathcal{C}'(\rho)\big(\mathcal{E}-\bar{\mathcal{E}}(\rho)\big)$ so that $W_{,\rho}(\rho,\mathcal{E}) = -F(\rho,\mathcal{E}) + \frac{1}{2}G(\rho,\mathcal{E})$. Then we have

$$\left|F(\rho,\mathcal{E}\mathbf{u}_a^h)-F(\rho,\mathcal{E}\mathbf{u}_b^h)\right| \le \left|\mathcal{E}(\mathbf{u}_a^h)-\mathcal{E}(\mathbf{u}_b^h)\right| \left|\mathcal{C}(\rho)\mathbb{1}e\right| \tag{3.12}$$

and

$$\begin{aligned}\left|F(\rho_a^h,\mathcal{E}(\mathbf{u}))-F(\rho_b^h,\mathcal{E}(\mathbf{u}))\right| \le{} & \left|m(\rho_a^h)-m(\rho_b^h)\right| \left|\mathcal{E}(\mathbf{u}) : (\mathcal{C}^M-\mathcal{C}^P)\mathbb{1}e\right| + \\ & \left|\rho_a^h-\rho_b^h\right| \left|\mathbb{1} : \mathcal{C}^P\mathbb{1}\right| e^2 + \\ & \left|\rho_a^h m(\rho_a^h)-\rho_b^h m(\rho_b^h)\right| \left|\mathbb{1} : (\mathcal{C}^M-\mathcal{C}^P)\mathbb{1}\right| e^2.\end{aligned} \tag{3.13}$$

Furthermore it holds that

$$\begin{aligned}\left|G(\rho_a^h,\mathcal{E}(\mathbf{u}))-G(\rho_b^h,\mathcal{E}(\mathbf{u}))\right| \le{} & \left|m'(\rho_a^h)-m'(\rho_b^h)\right| \left|\mathcal{E}(\mathbf{u}) : (\mathcal{C}^M-\mathcal{C}^P)\mathcal{E}(\mathbf{u})\right| + \\ & 2\left|\rho_a^h m'(\rho_a^h)-\rho_b^h m'(\rho_b^h)\right| \left|\mathcal{E}(\mathbf{u}) : (\mathcal{C}^M-\mathcal{C}^P)\mathbb{1}e\right| + \\ & \left|(\rho_a^h)^2 m'(\rho_a^h)-(\rho_b^h)^2 m'(\rho_b^h)\right| \left|\mathbb{1} : (\mathcal{C}^M-\mathcal{C}^P)\mathbb{1}\right| e^2\end{aligned} \tag{3.14}$$

and

$$\begin{aligned}\left|G(\rho,\mathcal{E}(\mathbf{u}_a^h))-G(\rho,\mathcal{E}(\mathbf{u}_b^h))\right| \le{} & \left|(\mathcal{E}(\mathbf{u}_a^h)-\mathcal{E}(\mathbf{u}_b^h)) : \mathcal{C}'(\rho)(\mathcal{E}(\mathbf{u}_a^h)+\mathcal{E}(\mathbf{u}_b^h))\right| + \\ & 2\left|\mathcal{E}(\mathbf{u}_a^h)-\mathcal{E}(\mathbf{u}_b^h)\right| \left|\mathcal{C}'(\rho)\bar{\mathcal{E}}(\rho)\right|.\end{aligned} \tag{3.15}$$

Combining (3.12)–(3.15), the assumptions on m and the L^∞-bounds on ρ_a^h, ρ_b^h, $\mathcal{E}(\mathbf{u}_a^h)$ and $\mathcal{E}(\mathbf{u}_b^h)$ we conclude

$$\left|W_{,\rho}(\rho_a^h,\mathcal{E}(\mathbf{u}_a^h))-W_{,\rho}(\rho_b^h,\mathcal{E}(\mathbf{u}_b^h))\right| \le c(\left|\mathcal{E}(\mathbf{u}_a^h)-\mathcal{E}(\mathbf{u}_b^h)\right| + \left|\rho_a^h-\rho_b^h\right|). \tag{3.16}$$

Uniqueness of the concentrations. Substracting the respective equations from each other we get

$$\left(\frac{\rho_a^h-\rho_b^h}{\tau_n},\varphi^h\right)^h = -\left(\nabla w_a^h-\nabla w_b^h,\nabla\varphi^h\right), \tag{3.17}$$

$$\begin{aligned}\left(w_a^h-w_b^h,\varphi^h\right)^h ={} & \left(\psi'(\rho_a^h)-\psi'(\rho_b^h),\varphi^h\right)^h + \gamma\Big(\nabla\rho_a^h-\nabla\rho_b^h,\nabla\varphi^h\Big) \\ & + \left(W_{,\rho}(\rho_a^h,\mathcal{E}(\mathbf{u}_a^h))-W_{,\rho}(\rho_b^h,\mathcal{E}(\mathbf{u}_b^h)),\varphi^h\right).\end{aligned} \tag{3.18}$$

Choosing $\varphi^h = \Delta_h^{-1}(\rho_a^h-\rho_b^h)$ in (3.17) and $\varphi^h = \rho_a^h-\rho_b^h$ in (3.18) and eliminating $\left(w_a^h-w_b^h,\rho_a^h-\rho_b^h\right)^h$ results in

$$\left(\frac{\rho_a^h-\rho_b^h}{\tau_n},\Delta_h^{-1}(\rho_a^h-\rho_b^h)\right)^h = \left(\psi'(\rho_a^h)-\psi'(\rho_b^h),\rho_a^h-\rho_b^h\right)^h + \gamma\left\|\nabla\rho_a^h-\nabla\rho_b^h\right\|_{L^2(\Omega)}^2$$

$$+\left(W_{,\rho}(\rho_a^h,\mathcal{E}(\mathbf{u}_a^h)) - W_{,\rho}(\rho_b^h,\mathcal{E}(\mathbf{u}_b^h)), \rho_a^h - \rho_b^h\right).$$

Using the fact that the cubic term in ψ' is monotone, (3.16) and (3.11) we get

$$-\frac{1}{\tau_n}\left(\rho_a^h - \rho_b^h, \Delta_h^{-1}(\rho_a^h - \rho_b^h)\right)^h + \gamma\left\|\nabla\rho_a^h - \nabla\rho_b^h\right\|_{L^2(\Omega)}^2 \le \frac{c}{h^{\frac{d}{2}}}\left\|\rho_a^h - \rho_b^h\right\|_{L^2(\Omega)}^2.$$

From the definition of Δ_h^{-1} and Young's inequality we have $\left\|\rho_a^h - \rho_b^h\right\|_{L^2(\Omega)}^2 \le \frac{1}{2\delta}\left\|\nabla\Delta_h^{-1}(\rho_a^h - \rho_b^h)\right\|_{L^2(\Omega)}^2 + \frac{\delta}{2}\left\|\nabla(\rho_a^h - \rho_b^h)\right\|_{L^2(\Omega)}^2$ for any $\delta > 0$ and thus

$$-\frac{1}{\tau_n}\left(\rho_a^h - \rho_b^h, \Delta_h^{-1}(\rho_a^h - \rho_b^h)\right)^h + \left(\gamma - \frac{c\delta}{2h^{\frac{d}{2}}}\right)\left\|\nabla\rho_a^h - \nabla\rho_b^h\right\|_{L^2(\Omega)}^2 \le \frac{c}{2\delta h^{\frac{d}{2}}}\left\|\nabla\Delta_h^{-1}(\rho_a^h - \rho_b^h)\right\|_{L^2(\Omega)}^2.$$

Choosing some $\delta < \frac{2\gamma h d^{\frac{d}{2}}}{c}$ and using

$$-\left(\rho_a^h - \rho_b^h, \Delta_h^{-1}(\rho_a^h - \rho_b^h)\right)^h = \left\|\nabla\Delta_h^{-1}(\rho_a^h - \rho_b^h)\right\|_{L^2(\Omega)}^2$$

we gather

$$\frac{1}{\tau_n}\left\|\nabla\Delta_h^{-1}(\rho_a^h - \rho_b^h)\right\|_{L^2(\Omega)}^2 \le \frac{c}{2\delta h^{\frac{d}{2}}}\left\|\nabla\Delta_h^{-1}(\rho_a^h - \rho_b^h)\right\|_{L^2(\Omega)}^2.$$

For $\tau_n < \frac{4\gamma h^d}{c^2}$ this can only hold if $\rho_a^h = \rho_b^h$. From this the equalities $w_a^h = w_b^h$ and $\mathbf{u}_a^h = \mathbf{u}_b^h$ follow immediately. $\square$

4. CONVERGENCE OF THE DISCRETIZED MODEL

We consider two ways to extend the sequences of solutions ρ_n^h, w_n^h and $\mathbf{u}_n^h$ for $n = 1, \ldots, N$ to functions in $L^\infty(0,T;H^{1,2}(\Omega))$ and $L^\infty(0,T;(H^{1,2}(\Omega))^d)$ respectively. By ρ^h, w^h and $\mathbf{u}^h$ we denote the piecewise constant, right continuous extension given by

$$\begin{aligned}
\rho^h(.,t) &:= \rho_n^h(.) && \text{for } t_{n-1} < t \le t_n,\\
w^h(.,t) &:= w_n^h(.) && \text{for } t_{n-1} < t \le t_n,\\
\mathbf{u}^h(.,t) &:= \mathbf{u}_n^h(.) && \text{for } t_{n-1} < t \le t_n.
\end{aligned}$$

In addition we make use of the piecewise affine extension

$$\begin{aligned}
\bar{\rho}^h(.,t) &:= \beta\rho_{n-1}^h(.) + (1-\beta)\rho_n^h(.),\\
\bar{w}^h(.,t) &:= \beta w_{n-1}^h(.) + (1-\beta)w_n^h(.),\\
\bar{\mathbf{u}}^h(.,t) &:= \beta\mathbf{u}_{n-1}^h(.) + (1-\beta)\mathbf{u}_n^h(.)
\end{aligned}$$

with $t = \beta t_{n-1} + (1-\beta)t_n$ and $0 \le \beta \le 1$.

Now we prove the following theorem

Theorem 1 (Convergence of discrete solutions)**.** *Assume that $\rho_0^h \in V^h$ are such that $\rho_0^h \to \rho_0$ in $H^1(\Omega)$ and let $(\rho^h, w^h, \mathbf{u}^h)$ be a solution of the discrete scheme (3.2)-(3.4) for $h \to 0$ und $\tau \to 0$ which are obtained by minimizing E^n. Then there is a subsequence with*

- *$\rho^h \to \rho$ pointwise almost everywhere, in $L^\infty(0,T;L^2(\Omega))$ and in $L^2(\Omega_T)$,*
- *$w^h \rightharpoonup w$ weakly in $L^2(0,T;H^{1,2}(\Omega))$,*
- *$\mathbf{u}^h \to \mathbf{u}$ pointwise almost everywhere, in $L^2(0,T;(H^{1,2}(\Omega))^d)$ and in $L^2(\Omega_T)$,*

where ρ and $\mathbf{u}$ solve (2.6)-(2.7), in the following weak sense:

(i)

$$-\int_{\Omega_T} \partial_t \xi (\rho - \rho_0) + \int_{\Omega_T} \nabla w \cdot \nabla \rho = 0$$

for all $\xi \in H^{1,2}(0,T;H^{1,2}(\Omega))$ with $\xi(T) = 0$.

(ii)

$$\int_{\Omega_T} w\, \xi = \int_{\Omega_T} [\gamma \nabla \rho \cdot \nabla \rho + \psi'(\rho)\, \xi + W_{,\rho}(\rho, \mathcal{E}(u))\, \xi]$$

for all $\xi \in L^2(0,T;H^{1,2}(\Omega)) \cap L^\infty(\Omega_T)$, and

(iii)

$$\int_{\Omega_T} C(\rho)(\mathcal{E}(u) - \bar{\mathcal{E}}(\rho)) : \mathcal{E}(\eta) = 0$$

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

Remark 1. Essential in the proof will be the fact that we can derive an energy decay property for solutions obtained by minimizing E^n. This property is not known for general solutions of (3.2)–(3.4). Let us point out that if the time-step restriction $\tau \le C_u h^2$ is fulfilled and if the triangulations are uniform we know from Section 3 that there is only one discrete solution which then of course fulfills the energy decay property.

Proof. The solution $\rho_n^h, \mathbf{u}_n^h$ of the n-th step of the discrete scheme minimizes E^n. So comparing the pair $\rho_n^h, \mathbf{u}_n^h$ with $\rho_{n-1}^h, \mathbf{u}_{n-1}^h$ we have $E^n(\rho_n^h, \mathbf{u}_n^h) \le E^n(\rho_{n-1}^h, \mathbf{u}_{n-1}^h)$ from which we gather that

$$E(\rho_n^h, \mathbf{u}_n^h) + \frac{1}{2\tau_n} \left\| \nabla \Delta_h^{-1} (\rho_n^h - \rho_{n-1}^h) \right\|_{L^2(\Omega)}^2 \le E(\rho_{n-1}^h, \mathbf{u}_{n-1}^h). \tag{4.1}$$

From(4.1) and

$$\frac{1}{2\tau_n} \left\| \nabla \Delta_h^{-1} (\rho_n^h - \rho_{n-1}^h) \right\|_{L^2(\Omega)}^2 = -\frac{\tau_n}{2} \left(\frac{\rho_n^h - \rho_{n-1}^h}{\tau_n}, w_n^h \right)^h = \frac{1}{2} \int_{t_{n-1}}^{t_n} \left\| \nabla w^h(t,.) \right\|_{L^2(\Omega)}^2$$

we gather

$$E(\rho^h(t,.),\mathbf{u}^h(t,.))+\frac{1}{2}\int\limits_0^T \left\|\nabla w^h(t,.)\right\|_{L^2(\Omega)}^2\,dt\le E(\rho_0^h,\mathbf{u}^h{}_0),\tag{4.2}$$

where $\mathbf{u}_0^h$ is the solution to (3.4) with $n=0$. Using the fact that $\int\limits_\Omega \rho^h(.,t)$ is preserved, the positivity of ψ we can use the inequalities of Poincaré and Korn to obtain: There is a $C>0$, depending on $\|\rho_0\|_{H^{1,2}(\Omega)}$, such that

$$\sup_{t\in[0,T]}\left\{\left\|\rho^h(.,t)\right\|_{H^{1,2}(\Omega)}+\left\|\mathbf{u}^h(.,t)\right\|_{H^{1,2}(\Omega)}\right\}\le C.\tag{4.3}$$

Futhermore we have that w^h is bounded in $L^2(\Omega\times[0,T])$ and that

$$\sup_{t\in[0,T]}\int\limits_\Omega \psi(\rho^h)\,dx\le C.\tag{4.4}$$

In order to control the variations in time we consider the piecewise affine extension $\bar\rho^h$. From (3.2) we have

$$\left(\partial_t\bar\rho^h(t),\varphi^h\right)^h+\left(\nabla w_n^h,\nabla\varphi^h\right)=0\qquad\qquad \forall\varphi^h\in V^h.\tag{4.5}$$

Testing with $\varphi^h=\bar\rho^h(s_2)-\bar\rho^h(s_1)$ for arbitrary $0\le s_1<s_2\le T$ yields

$$\left|\bar\rho^h(s_2)-\bar\rho^h(s_1)\right|_h^2+\int\limits_{s_1}^{s_2}\left(\nabla w^h(t),\nabla\bar\rho^h(s_2)-\nabla\bar\rho^h(s_1)\right)\,dt=0.$$

From (4.3) we see that $\rho_n^h(.,t)$ is bounded in $H^{1,2}(\Omega)$ and thus $\bar\rho^h$ in $L^\infty((0,T);H^{1,2}(\Omega))$. Using Hölders inequality we gather

$$\begin{aligned}\left|\bar\rho^h(s_2)-\bar\rho^h(s_1)\right|_h^2&\le C\left\|\bar\rho^h\right\|_{L^\infty(H^{1,2}(\Omega))}\int\limits_{s_1}^{s_2}\left\|\nabla w^h(t)\right\|_{L^2(\Omega)}\,dt\\&\le C\left\|\bar\rho^h\right\|_{L^\infty(H^{1,2}(\Omega))}(s_2-s_1)^{\frac12}\left\|\nabla w^h\right\|_{L^2(\Omega_T)}.\end{aligned}$$

Therefore there is a constant $C>0$ such that

$$\left\|\bar\rho^h(s_2)-\bar\rho^h(s_1)\right\|_{L^2(\Omega)}\le C\left|s_2-s_1\right|^{\frac14}.\tag{4.6}$$

In other words we have the uniform continuity of $\rho^h:[0,T]\to L^2(\Omega)$ with respect to time.

Arzelà-Ascolis theorem and the fact that $\bar\rho^h(.,t)$ is uniformly bounded in $H^1(\Omega)$ now guarantees the existence of a converging subsequence

$$\bar\rho^h\to\rho^*\qquad\qquad \text{in}\quad C^{0,\alpha}(0,T;L^2(\Omega))$$

for any $0<\alpha<\frac14$.

For $t \in [0,T]$, arbitrary n and $\beta \in (0,1)$ such that $t = \beta t_{n-1} + (1-\beta)t_n$ we have:

$$\begin{aligned}\left\|\rho^h(.,t) - \bar{\rho}(.,t)\right\|_{L^2(\Omega)} &= \left\|\rho_n^h - \beta\rho_{n-1}^h - (1-\beta)\rho_n^h\right\|_{L^2(\Omega)} \\ &= \beta\left\|\rho_n^h - \rho_{n-1}^h\right\|_{L^2(\Omega)} \\ &\leq C\tau_n^{\frac{1}{4}} \to 0.\end{aligned}$$

This ensures $\rho^h \to \rho^*$ in $L^\infty(0,T;L^2(\Omega))$ and convergence of ρ^h in $L^2(\Omega_T)$. Furthermore we have pointwise convergence almost everywhere along a subsequence.

Concerning the nonlinearity we have for any $\delta > 0$ a constant C_δ

$$\int\limits_E \left|\psi'(\rho^h)\right| \, dx \leq \delta \int\limits_E \left|\psi(\rho^h)\right| \, dx + C_\delta \left|E\right| \leq \delta C + C_\delta \left|E\right|$$

and thus $\int_E \left|\psi'(\rho^h)\right| \, dx \to 0$ uniformly in h and τ if $|E| \to 0$ where $|E|$ denotes the measure of $E \subset \Omega \times (0,T)$. Then Vitalis theorem yields $\psi'(\rho^h) \to \psi'(\rho^*)$ in $L^1(\Omega \times (0,T))$.

From(4.3) only weak convergence

$$\mathbf{u}^h \rightharpoonup \mathbf{u}^* \qquad \text{in} \quad L^2(0,T;(H^{1,2}(\Omega))^d)$$

along a subsequence follows immediately. In order to get strong convergence we make use of Cléments interpolation operator Π. It holds (see[4])

$$\lim_{h\to 0} \|\mathbf{u}^* - \Pi\mathbf{u}^*\|_{H^{1,2}(\Omega)} = 0. \tag{4.7}$$

Testing (3.4) with $\mathbf{u}^h - \Pi\mathbf{u}^* \in (V^h)^d$ and integration time yields

$$0 = \int\limits_0^T \left\langle \mathcal{E}(\mathbf{u}^h) - \bar{\mathcal{E}}(\rho^h), \mathcal{E}(\mathbf{u}^h - \Pi\mathbf{u}^*)\right\rangle_{\mathcal{C}(\rho^h)} dt. \tag{4.8}$$

Then we have

$$\begin{aligned}&d_0 \int\limits_0^T \left\|\mathcal{E}(\mathbf{u}^h - \mathbf{u}^*)\right\|_{L^2(\Omega)}^2 dt \leq \\ &\leq 2d_0 \int\limits_0^T \left\|\mathcal{E}(\mathbf{u}^h - \Pi\mathbf{u}^*)\right\|_{L^2(\Omega)}^2 + \|\mathcal{E}(\Pi\mathbf{u}^* - \mathbf{u}^*)\|_{L^2(\Omega)}^2 \, dt \\ &\leq 2\int\limits_0^T \left\langle \mathcal{E}(\mathbf{u}^h) - \bar{\mathcal{E}}(\rho^h) - \mathcal{E}(\Pi\mathbf{u}^*) + \bar{\mathcal{E}}(\rho^h), \mathcal{E}(\mathbf{u}^h - \Pi\mathbf{u}^*)\right\rangle_{\mathcal{C}(\rho^h)} dt \\ &\quad + 2d_0 \int\limits_0^T \|\mathcal{E}(\Pi\mathbf{u}^* - \mathbf{u}^*)\|_{L^2(\Omega)}^2 \, dt\end{aligned}$$

$$\overset{(4.8)}{=} -2\int_0^T \left\langle \mathcal{E}(\Pi\mathbf{u}^*) - \bar{\mathcal{E}}(\rho^h), \mathcal{E}(\mathbf{u}^h - \Pi\mathbf{u}^*)\right\rangle_{\mathcal{C}(\rho^h)} dt +$$

$$+ 2d_0 \int_0^T \|\mathcal{E}(\Pi\mathbf{u}^* - \mathbf{u}^*)\|^2_{L^2(\Omega)}\, dt$$

$$= -2\int_0^T \left(\mathcal{E}(\mathbf{u}^h - \Pi\mathbf{u}^*)\right) : \mathcal{C}(\rho^h)\left(\mathcal{E}(\Pi\mathbf{u}^*) - \bar{\mathcal{E}}(\rho^h)\right) dt +$$

$$+ 2d_0 \int_0^T \|\mathcal{E}(\Pi\mathbf{u}^* - \mathbf{u}^*)\|^2_{L^2(\Omega)}\, dt.$$

Consider the first summand on the right hand side. The first factor converges weakly to zero and the second factor strongly to $\mathcal{C}(\rho^*)\left(\mathcal{E}(\mathbf{u}^*) - \bar{\mathcal{E}}(\rho^*)\right)$. Hence the first summand vanishes for $h \to 0$ and so does the second summand because of (4.7). With Korn's inequality we deduce strong convergence of $\mathbf{u}^h$ in $L^2(0,T;(H^{1,2}(\Omega))^d)$. This implies that after possibly extracting another subsequence for almost any $t \in [0,T]$ we have $L^2(\Omega)$ convergence $\mathcal{E}(\mathbf{u}^h(t,.)) \to \mathcal{E}(\mathbf{u}^*(t,.))$. We now show that also the elastic contribution to the chemical potential

$$W_{,\rho}(\rho_n^h, \mathcal{E}(\mathbf{u}_n^h)) = -e\mathbb{1} : \mathcal{C}(\rho_n^h)\left(\mathcal{E}(\mathbf{u}_n^h) - \bar{\mathcal{E}}(\rho_n^h)\right) + \left(\left(\mathcal{E}(\mathbf{u}_n^h) - \bar{\mathcal{E}}(\rho_n^h)\right) : \mathcal{C}'(\rho_n^h)\left(\mathcal{E}(\mathbf{u}_n^h) - \bar{\mathcal{E}}(\rho_n^h)\right)\right) \tag{4.9}$$

converges in $L^1(\Omega)$ for almost any $t \in [0,T]$. The first summand in (4.9) can be bounded by

$$\begin{aligned}\left|e\mathbb{1} : \mathcal{C}(\rho_n^h)\left(\mathcal{E}(\mathbf{u}_n^h) - \bar{\mathcal{E}}(\rho_n^h)\right)\right| &\le \frac{1}{2}\left(\left|e\,\mathcal{C}(\rho_n^h)\mathbb{1}\right|^2 + \left|\mathcal{E}(\mathbf{u}_n^h) - \bar{\mathcal{E}}(\rho_n^h)\right|^2\right)\\ &\le c\left(\left|\mathcal{E}(\mathbf{u}_n^h)\right|^2 + \left|\rho_n^h\right|^2 + 1\right).\end{aligned}$$

Since $C'(r)$ is bounded there exists a constant $c > 0$ such that

$$\begin{aligned}\left|\left(\left(\mathcal{E}(\mathbf{u}_n^h) - \bar{\mathcal{E}}(\rho_n^h)\right) : \mathcal{C}'(\rho_n^h)\left(\mathcal{E}(\mathbf{u}_n^h) - \bar{\mathcal{E}}(\rho_n^h)\right)\right)\right| &\le c\left|\mathcal{E}(\mathbf{u}_n^h) - \bar{\mathcal{E}}(\rho_n^h)\right|^2\\ &\le 2c\left(\left|\mathcal{E}(\mathbf{u}_n^h)\right|^2 + \left|\rho_n^h\right|^2\right).\end{aligned}$$

With Lesbegues theorem it follows that $W_{,\rho}(\rho_n^h, \mathcal{E}(\mathbf{u}_n^h))$ converges in $L^2(0,T;L^1(\Omega))$ with limit $W_{,\rho}(\rho, \mathcal{E}(\mathbf{u}))$.

Testing (3.3) with $\varphi^h = 1$ yields (where $\mathcal{I}^n$ is the Lagrange interpolation operator and tr is the trace)

$$\int_\Omega w_n^h\, dx = \int_\Omega \mathcal{I}^n\left(\psi'(\rho_n^h)\right) - e\,\mathrm{tr}(\mathcal{S}_n^h)\, dx$$

$$+\int\limits_{\Omega}\left(\mathcal{E}(\mathbf{u}_n^h)-\bar{\mathcal{E}}(\rho_n^h)\right):\mathcal{C}'(\rho_n^h)\left(\mathcal{E}(\mathbf{u}_n^h)-\bar{\mathcal{E}}(\rho_n^h)\right)\,dx,$$

where the right hand side is uniformly bounded. From the generalized Poincaré inequality we gather that w^h is uniformly bounded in $L^2(0,T;H^{1,2}(\Omega))$. This implies the existence of a weakly converging subsequence

$$w^h \rightharpoonup w^* \qquad \text{in } L^2(0,T;H^{1,2}(\Omega)).$$

For $\zeta \in L^2(0,T;H^{1,2}(\Omega))$ with $\partial_t\zeta \in L^2(\Omega_T)$ and $\zeta(T)=0$ we obtain from (4.5) by choosing $\varphi^h(.)=\Pi\zeta(.,t_n)$, integration with respect to time and integration by parts

$$\int_{\Omega_T}(\bar{\rho}^h-\rho_0^h)\partial_t\Pi\zeta+\int_{\Omega_T}\nabla u^h\nabla\Pi\zeta=\mathcal{O}(h).$$

The $\mathcal{O}(h)$ appears since we replaced the discrete inner product $(.,.)^h$ by $(.,.)$. The convergence properties of $\bar{\rho}^h$, ρ_0^h, w^h and $\Pi\zeta$ then give that (i) holds. For the second term on the left hand side for example the strong convergence of $\nabla\Pi\zeta$ and the weak convergence of ∇w^h yields convergence of the product.

If we test the second equation with $\Pi\zeta$ we get

$$\begin{aligned}\left(w_n^h,\Pi\zeta\right)^h &= \left(\psi'(\rho_n^h),\Pi\zeta\right)^h+\gamma\Big(\nabla\rho_n^h,\nabla\Pi\zeta\Big)-e\left(\mathrm{tr}(\mathcal{S}_n^h),\Pi\zeta\right)\\ &\quad+\left(\left(\mathcal{E}(\mathbf{u}_n^h)-\bar{\mathcal{E}}(\rho_n^h)\right):\mathcal{C}'(\rho_n^h)\left(\mathcal{E}(\mathbf{u}_n^h)-\bar{\mathcal{E}}(\rho_n^h)\right),\Pi\zeta\right).\end{aligned}$$

Integration with respect to time and using the convergence properties obtained above give that we obtain (ii) in the limit $h\to 0$. To pass to the limit in the time integrated version of the third equation (3.4) we make use of the fact that $\left|\mathcal{C}(\rho_n^h)\left(\mathcal{E}(\mathbf{u}_n^h)-\bar{\mathcal{E}}(\rho_n^h)\right)\right|\le c\left(\left|\mathcal{E}(\mathbf{u}_n^h)\right|+\left|\rho_n^h\right|+1\right)$, the strong convergence of ρ^h and $\mathcal{E}(\mathbf{u}^h)$ in $L^2(\Omega_T)$ and almost everywhere and Lebesgue's theorem. □

5. NUMERICAL RESULTS

In this section we present some numerical results showing a variety of effects associated with and caused by the presence of elasticity. The calculations have been performed using the θ-scheme [1, 19] a more complicated but numerically more stable time discretization (see [12, 22] for the application of this scheme to the Cahn-Hilliard and the Cahn-Larché equation). Of course we checked that the scheme based on the implicit Euler discretization exhibits the same qualitative effects albeit with more computational effort. To solve the resulting nonlinear discrete problems we used Newton's method where we solved the linear systems with the help of the BICG and GMRES algorithms.

The domain of calculation has been the unit square and we took $\gamma = 10^{-5}$. We assumed cubic symmetry (see [14]) and as elastic parameters we chose in the case of inhomogeneous elasticity $C_{1111}=4$, $C_{1122}=2$, $C_{1212}=20$ for the one phase and $C_{1111}=1$, $C_{1122}=\frac{1}{2}$, $C_{1212}=5$ for the other (all other entries in the elasticity tensor C are determined by symmetry) and we set $e=0.1$. In the case of homogeneous elasticity we took the first set of parameters for C.

In the calculations in the Figures 4, 5 and 7 periodic boundary conditions were imposed and in Figure 5 the domain of calculation was copied once in order to improve the visual effect.

Alignment of interfaces. In the case of a elasticity tensor with cubic anisotropy one observes an alignment of the interfaces with the coordinate axis as can be seen in Figure 2.

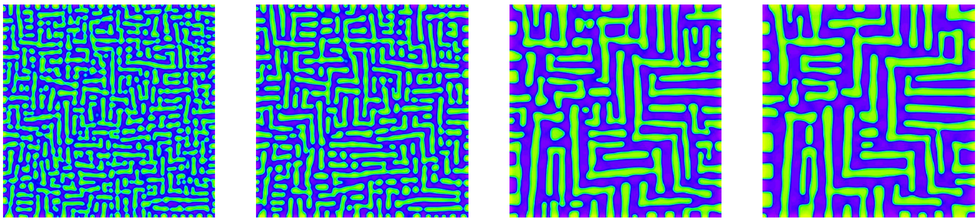


FIGURE 2. Alignment of interfaces driven by homogeneous, anisotropic elasticity

Alignment of particles. In the case of inhomogeneous elasticity one observes that particles align to each other and in strong contrast to the standard Cahn-Hilliard system do not merge when close but instead repell each other (see Figure 3. In Figure 4 an evolution with two initially ball shaped particles whose distance is smaller than their radius is shown. Instead of the merging one observes anisotropic deformation of the particles, alignment to each other and a movement such that the particles have maximum distance to each other given the periodic boundary conditions.

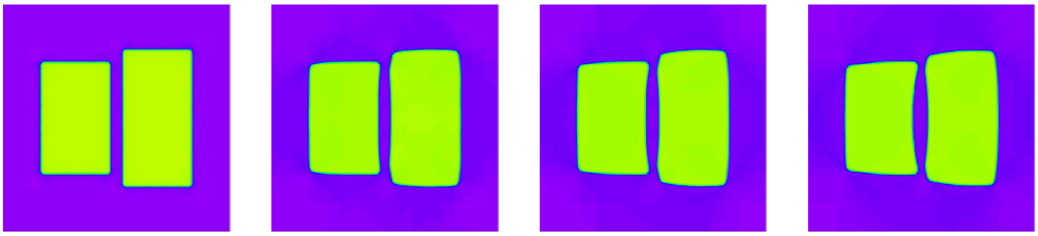


FIGURE 3. Repulsion of two particles due to anisotropic elasticity

The same effect is shown in a more complicated situation in Figure 5. Here the initial condition is given by some randomly positioned ball shaped particles of the same size. Again the area of computation has been the unit square and periodic boundary conditions have been imposed. In order to show the alignment effect, the picture has been copied once.

In Figure 1 the initial data have been a randomly perturbed constant and so that in the first phase spinodal decomposition takes places. Again one can see the anisotropic particle shapes and the alignment of particles.

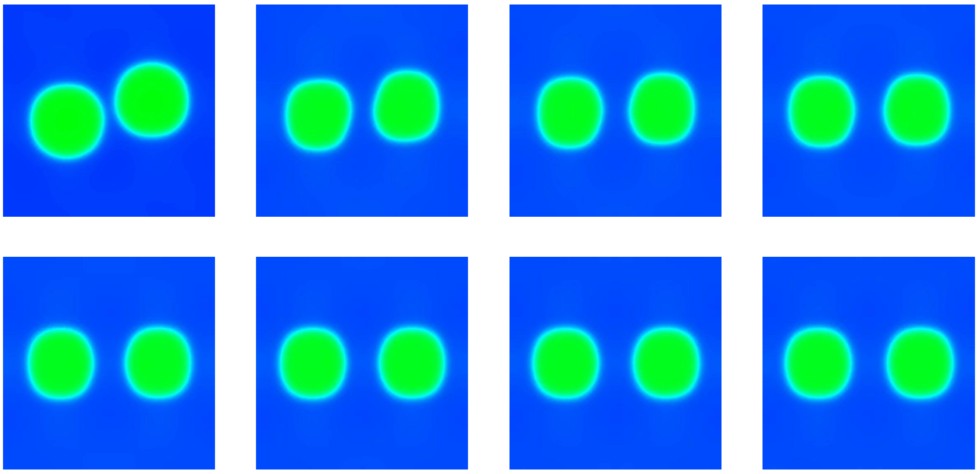
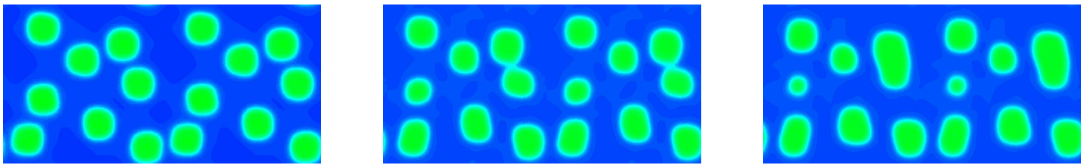
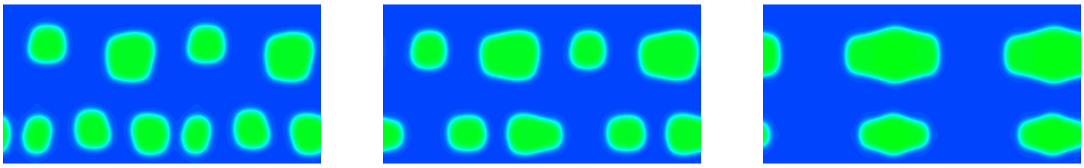


FIGURE 4. Alignment and repulsion of particles with inhomogeneous, anisotropic elasticity



(a) t=0.005 (b) t=0.125 (c) t=0.25

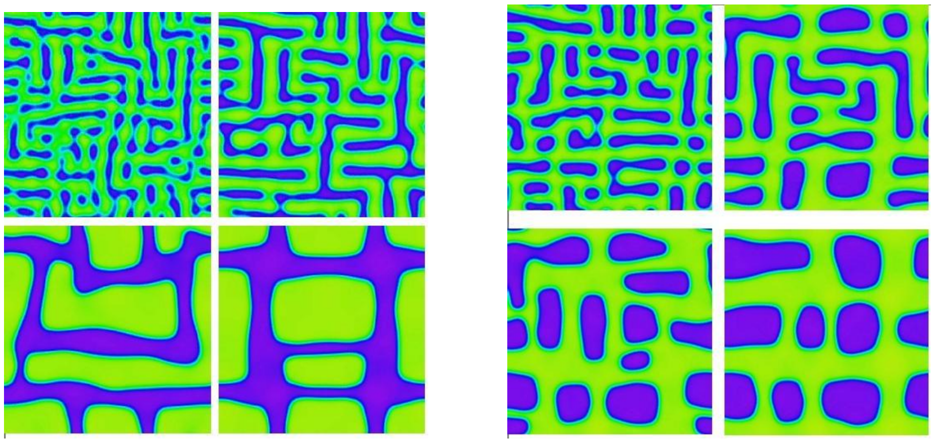


(d) t=0.5 (e) t=1 (f) t=2

FIGURE 5. Alignment and repulsion of particles with inhomogeneous, anisotropic elasticity

Relation of matrix and particle phase. The Cahn-Hilliard model is symmetric with respect to the phases: The evolution starting from $-\rho_0$ is apart from the exchange of the phases identical to the evolution starting from ρ_0. Which phase forms the particles and which one forms the surrounding matrix is determined by the mass ratio. From the minimization of the interfacial region it is clear that the phase with the lower mass fraction forms the particles.

In the Cahn-Larché model the impact of inhomogeneous elasticity may alter this behaviour. If the difference of the elastic moduli is not to small it is always



(a) light: hard, dark: soft (b) light: soft, dark: hard

Figure 6. Evolutions with switched elasticity tensors for the pure phases.

the elastically harder phase that forms the particle. In Figure 6 two evolutions with identical initial values are depicted. The only difference is that the values of the elasticity tensors for the pure phases $\mathcal{C}^M$ and $\mathcal{C}^P$ are switched. Thus, in Figure 6(a) the phase with the higher mass fraction forms the particles. Here again one can observe anisotropic particle shapes and alignment of particles.

In Figure 7 the initial value has been chosen to feature particles of the elastically softer phase. In addition periodic boundary conditions were imposed. In the course of the evolution the roles of particle and matrix phase switch.

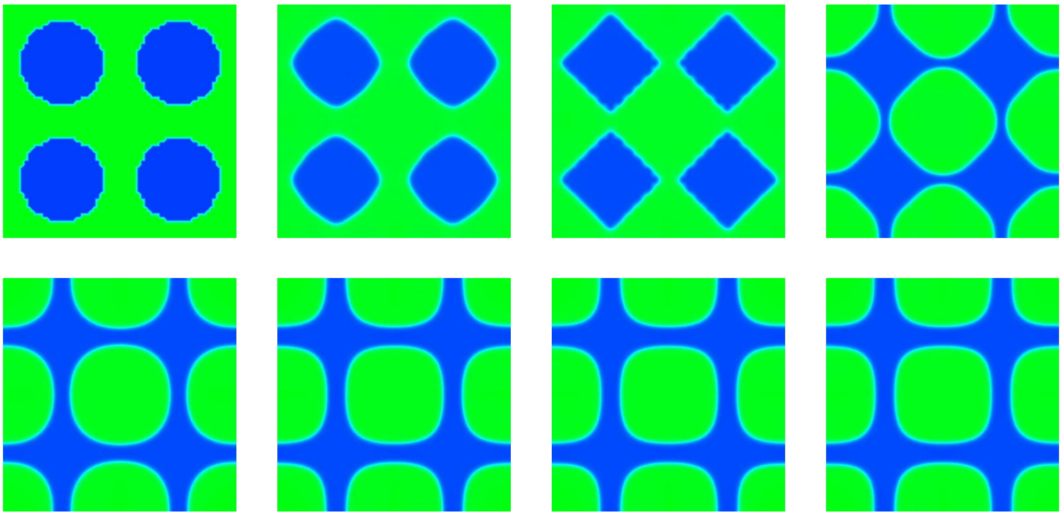


Figure 7. Switch from matrix to particle phase.

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