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On the solvability of a two scale model for liquid phase epitaxy with elasticity

Christof Eck [*], Michael Kutter [†]

Abstract

We study a two-scale model for liquid phase epitaxy with elasticity. The model has been derived via homogenization by formal asymptotic expansion in [10]. It consists of a macroscopic Navier–Stokes–System and a macroscopic convection-diffusion equation for the transport of matter in the liquid, and a microscopic problem that combines a phase-field approximation of a BCF-model, a Stokes system and an elasticity system for the growth and the elastic deformation of the solid film. For each of these problems we prove the existence and uniqueness of solutions under the assumption that the coupling data are given, sufficiently regular functions. These results are a first step in the proof of the existence of solutions to the full model via a suitable fixpoint argument, applied to the composition of appropriate solution operators, as it has been done for a corresponding model without elasticity in [8].

KEYWORDS: liquid phase epitaxy, homogenization, multi-scale model, existence of solutions
MSC: 35K55, 35R35, 80M40

1 Introduction

Epitaxy is a technical process for the production of thin films and layers. The main mechanism is the deposition of single molecules on the growing film, where these molecules diffuse until they reach a mono-molecular step and incorporate to the solid material. Applications of epitaxy are the production of solar cells, integrated circuits, lasers, and light emitting diodes. The technical relevance of epitaxy comes from the possibility to generate microstructures of different morphologies as e.g. steps, islands, and spirals in the produced solid film. The classical model for epitaxy, in particular molecular beam epitaxy, is the Burton–Cabrera–Frank model (BCF–model) [2]. This model resolves the single mono-molecular layers that contribute to the growing solid and uses a continuum mechanical description of the surface diffusion via a diffusion equation. The boundaries of the mono-molecular steps are described by a free boundary with appropriate boundary conditions. An alternative description to this free boundary problem are phase field models [13], where the boundaries of the mono-molecular steps are approximated by a diffuse phase boundary that is described by an additional phase field, [21]. There are also purely continuum mechanical models; the simplest type of such a models describes the height of the solid film via a differential equation of fourth order [24]. Sometimes also purely atomistic models are used in corresponding Monte–Carlo–simulations [22]; due to the huge number of unknowns these models need they are, however, only applicable for very small length scales.
In liquid phase epitaxy the molecules that contribute to the growing film are solved in a liquid and transported to the solid film by convection and diffusion. Models for liquid phase epitaxy combine an appropriate model for epitaxy with transport equations in the liquid via suitable boundary conditions, see e.g. [8]. It is

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known that some microstructures that arise in liquid phase epitaxy are generated by instabilities in the elastic deformation. In order to model such effects, it is necessary to also include elasticity equations for the deformation of the solid film into the model, see e.g. [10].
The microstructures that typically arises in epitaxy makes the direct numerical simulation of the process for technically relevant length scales cumbersome and in some cases even impossible, because a corresponding numerical grid has to resolve the full microstructure. More suitable models for such a situation can be obtained by the application of homogenization techniques, see e.g. [7]. Since the microstructure is a priori unknown, homogenization does not lead to a purely macroscopic model, but to a two- or multi-scale model that combines macroscopic equations with microscopic problems for the computation of the microstructure.
In this paper we consider a two-scale model for liquid phase epitaxy with elasticity that shall be suitable for the simulation of problems with large length scales. This model is derived in [10] by homogenization via formal asymptotic expansion in combination with a matched asymptotic expansion close to the solid film. It is composed of a macroscopic problem that consists of a Navier-Stokes system and a convection-diffusion equation for the transport processes in the liquid and a family of microscopic problems that describe the growth of the solid film, its elastic deformation and the coupling of elastic deformations to the macroscopic equations. The microscopic problems consist of a phase field version of the BCF–model, an elasticity system, and a Stokes system on a semi–infinite domain. The Stokes system arises in the inner expansion of the matched asymptotic expansion, it couples the elasticity equations to the macroscopic Navier–Stokes equations. A corresponding model for liquid phase epitaxy without elasticity has already been analyzed in [8]. The inclusion of elasticity makes the model much more challenging, because the domains for the elasticity equations and the Stokes system depend on the phase field. Our final aim is the proof of existence and uniqueness of a solution. In this paper we analyze the single parts of the model with coupling data considered as given functions. The results presented here are necessary for the proof of the existence of solutions to the full two-scale model by the application of a fixed point theorem to the composition of the corresponding solution operators, as it has been done in [8] for the model without elasticity.

2 The two-scale model

We consider a domain $Q \in \mathbb{R}^3$ which has the form of a container, see Figure 1. The bottom of Q is denoted by $S_0 := \{x \in \overline{Q} \,|\, x_3 = 0\}$. The solid film grows on S_0, the domain occupied by this film is denoted by $Q_S = Q_S(t)$; it depends on the time t. The liquid domain is $Q_L = Q \setminus \overline{Q_S}$, the interface between Q_L and Q_S is denoted by S. Both Q_L and S depend on the time. The interface S is parameterized by a height function h,

$$S(t) = \{x + h(x,t)e_3 \,|\, x \in S_0\}$$

with unit vector e_3. Then the domains Q_l and Q_s and the interface Γ are given by

$$\begin{aligned}
Q_l(t,x) &= \{y \in \mathbb{R}^3 \mid (y_1,y_2) \in Y,\ y_3 > h_A\Phi(t,x,y_1,y_2)\},\\
Q_s(t,x) &= \{y \in \mathbb{R}^3 \mid (y_1,y_2) \in Y,\ 0 < y_3 < h_A\Phi(t,x,y_1,y_2)\}, \text{ and}\\
\Gamma(t,x) &= \{y \in \mathbb{R}^3 \mid (y_1,y_2) \in Y,\ y_3 = h_A\Phi(t,x,y_1,y_2)\}.
\end{aligned}$$

Here h_A is the height of a mono-molecular layer and Φ denotes the phase field that represents the number of mono-molecular steps. Hence $h_A\Phi$ represents the height of the solid film.
We consider a two-scale model for liquid phase epitaxy that covers the transport processes in the liquid solution, the mechanical deformation in the solid layer and the growth of the solid film. This model is derived by a formal asymptotic expansion from a corresponding model for a problem with given scale parameter ε; it corresponds to a (formal) limit $\varepsilon \to 0$ of this model. For the derivation of this model and a more detailed description we refer to [10]. In our model we replace the BCF–model in [10] by a corresponding phase field model. The macroscopic variable is denoted by $x \in Q$, the microscopic by $y \in Y \times \mathbb{R}_+$ or by $y \in Y$, where Y is a two-dimensional periodicity cell, e.g. $[0,1]^2$. The model is composed of

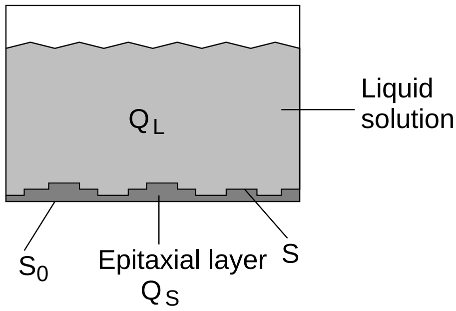

Figure 1: Liquid Phase Epitaxy

- A macroscopic Navier-Stokes system and a macroscopic convection-diffusion equation for the transport in the liquid,

$$\begin{aligned} \operatorname{div} V &= 0, \\ \partial_t V + (V \cdot \nabla)V - \eta \Delta V + \nabla P &= 0, \end{aligned} \tag{1}$$

$$\partial_t C^V + V \cdot \nabla C^V - D_V \Delta C^V = 0. \tag{2}$$

  Here V denotes the velocity field, P the pressure, C^V the concentration of molecules in the solution, D_V is a diffusion constant and η the viscosity of the fluid. The variables V, P, and C^V are denoted by capital letters in order to distinguish them from the corresponding variables of the microscopic problems. For the fluid velocity we have the boundary condition

$$V = 0 \text{ on } S_0. \tag{3}$$

  As a consequence the Navier-Stokes system decouples from the other equations. Therefore we may consider the velocity field V as given function.

- A microscopic Stokes system on $Q_l(t, x)$ that must be solved for every $x \in S_0$:

$$\begin{aligned} \operatorname{div}_y v &= 0, \\ -\eta \Delta_y v + \nabla_y p &= 0 \end{aligned} \tag{4}$$

  with microscopic velocity field v and microscopic pressure p. Here v denotes the term of order ε in the inner expansion of the homogenization procedure; the term of order 1 vanishes.

- A microscopic elasticity system to be solved for every $x \in S_0$ on the domain $Q_s(t, x)$,

$$-\operatorname{div}_y \sigma_y(u) = 0, \tag{5}$$

  with stress tensor $\sigma_y(u) = \mathbf{a} e_y(u)$ and linearized strain tensor $e_y(u) = \frac{1}{2}\left(\nabla_y u + (\nabla_y u)^\top\right)$. This system is complemented by a Dirichlet boundary condition

$$u = b \tag{6}$$

  for $y \in Y \times \{0\}$.

- A microscopic phase field model to be solved on Y for every $x \in S_0$,

$$\alpha \xi^2 \partial_t \Phi - \xi^2 \Delta_y \Phi + f'(\Phi) + q(c^S, u, \Phi) = 0, \tag{7}$$

$$\partial_t c^S + \varrho_S h_A \partial_t \Phi - D_S \Delta_y c^S = \frac{c^V}{\tau_V} - \frac{c^S}{\tau_S}. \tag{8}$$

Here Φ denotes the phase field and c^S the surface density of adatoms, measured by the mass of adatoms per unit area, D_S the diffusivity for the surface diffusion, ϱ_S the surface density of adatoms, α a time relaxation parameter, ξ describes the thickness of the diffuse interface and τ_V and τ_S the rates of adsorption and desorption of adatomes from and to the liquid solution. The function f is a multi-well potential with minima at integer values, e.g. $f(\Phi) = -\cos(2\pi\Phi)$, and

$$q(c^S, u, \Phi) = \frac{R\mathcal{T}\varrho_S}{c_{\mathrm{eq}}\gamma\beta}(c_{eq} - c^S) + \frac{h_A\varrho_S}{2c_{eq}\gamma\beta}\sigma_y(\mathcal{R}_\mu(u)) : e_y(\mathcal{R}_\mu(u)) \tag{9}$$

with gas constant R, temperature $\mathcal{T}$, equilibrium concentration c_{eq}, step stiffness γ, and a calibration parameter β. Here we use a regularisation $\mathcal{R}_\mu(u)$ in the density of elastic energy that arises in the phase field model.

- The coupling between the single parts of the model: The conservation of adatoms leads to

$$D_V \partial_{x_3} C^V|_{x_3=0} = -\left(\frac{\bar{c}^S}{\tau_S} - \frac{c^V}{\tau_V}\right) \quad \forall x \in S_0, \tag{10}$$

this relation serves as boundary condition for (2) on S_0. Here $\bar{c}^S(t,x) = \int_Y c^S(t,x,y)\ \mathrm{d}y$ is the microscopic mean value of c^S. The coupling between the microscopic and the macroscopic velocity and pressure is given by the equilibrium of forces

$$\begin{aligned} &\lim_{y_3\to\infty} \eta\left(\nabla_y v + (\nabla_y v)^\top\right) e_3 - p e_3 = \\ &\qquad \eta\left(\nabla_x V|_{x_3=0} + (\nabla_x V)^\top|_{x_3=0}\right) e_3 - P|_{x_3=0} e_3. \end{aligned} \tag{11}$$

On Γ, we have the condition

$$v = J_S^{-1}\left(\frac{1}{\varrho_V} - \frac{1}{\varrho_E}\right)\left(\frac{c^V}{\tau_V} - \frac{c^S}{\tau_S}\right) n_y \quad \text{for all } y \in \Gamma,\ x \in S_0, \tag{12}$$

due to the conservation of mass. The factor $J_S = \sqrt{1 + |\nabla h|^2}$ is the density of surface measure of S parametrized over S_0. The balance of forces between the liquid phase and the solid phase on Γ gives

$$\sigma_y(u) n_{yS} + \eta\left(\nabla_y v + (\nabla_y v)^\top\right) n_{yL} - p n_{yL} = 0, \quad \forall y \in \Gamma,\ x \in S_0. \tag{13}$$

Here n_{yS} and n_{yL} are outer normal vectors with respect to the corresponding domains Q_s for n_{yS} and Q_l for n_{yL}.

All mentioned variables are time dependent and thus considered on a time intervall $[0, T]$. Equations of parabolic type are supplemented by initial conditions. The microscopic problems are completed with periodic boundary conditions for $y \in \partial Y$.

3 The microscopic Stokes system

We consider (4), (11) and (12) with given data c^V, c^S, V and P. We prove the existence of a solution which satisfies

$$\lim_{y_3\to\infty} p = P|_{x_3=0},$$

and thus (11) is modified to

$$\lim_{y_3\to\infty} \left(\nabla_y v + (\nabla_y v)^\top\right) e_3 = \left(\nabla_x V|_{x_3=0} + (\nabla_x V)^\top|_{x_3=0}\right) e_3.$$

Due to the boundary condition $V(t,x) = 0$ for $x \in S_0$ we find $\partial_{x_1} V|_{x_3=0} = \partial_{x_2} V|_{x_3=0} = 0$ and with $\operatorname{div} V = 0$ we conclude $\partial_{x_3} V_3 = 0$. Thus, the right hand side of the above boundary equation is

$$a := \left.\begin{pmatrix} \partial_{x_3} V_1 \\ \partial_{x_3} V_2 \\ 0 \end{pmatrix}\right|_{x_3=0}.$$

We define

$$\tilde{v} := \chi(y_3) a\, y_3,$$

where χ is a smooth cut-off function with $\chi(y_3) = 0$ for $y_3 \leq M$ for a sufficiently large M, $0 \leq \chi(y_3) \leq 1$ and $\chi(y_3) = 1$ for y_3 sufficiently large. Obviously, we have

$$\lim_{y_3 \to \infty} \left(\nabla_y \tilde{v} + (\nabla_y \tilde{v})^\top \right) = a, \quad \operatorname{div} \tilde{v} = 0.$$

We further define the constant vector $\hat{v} = (0, 0, \hat{v}_3)^\top \in \mathbb{R}^3$ such that

$$\int_\Gamma \hat{v} \cdot n \, \mathrm{d}y = \int_\Gamma v_\Gamma \cdot n \, \mathrm{d}y,$$

i.e.

$$\hat{v}_3 := \frac{\int_\Gamma v_\Gamma \cdot n \, \mathrm{d}y}{\int_\Gamma n_3 \, \mathrm{d}y}.$$

For the moment, we introduce an artificial boundary $\hat{\Gamma} := \{y \in Q_l | y_3 = h_A \Phi(y_1, y_2) + K\}$, where the positive constant K is chosen such that $\chi(y_3) = 0$ for $y_3 \leq h_A \Phi(y_1, y_2) + K$ and $(y_1, y_2) \in Y$. The surface $\hat{\Gamma}$ is the upper boundary of the domain $Q_{lK}(t,x) := \{y \in Q_l | y_3 < h_A \Phi(y_1, y_2) + K\}$. In order to transform the inhomogeneous Dirichlet condition on Γ to a homogeneous one, we prove the following statement:

Lemma 3.1. *Let $v_\Gamma \in H^{1/2}_{\mathrm{per}}(\Gamma)$ and $Y = [0,1]^2$. Then, there exists a function $u \in [H^1_{\mathrm{per}}(Q_{lK})]^3$ such that $u|_\Gamma = v_\Gamma - \hat{v}$, $u|_{\hat{\Gamma}} = 0$ and $\operatorname{div} u = 0$. Furthermore,*

$$\|u\|_{H^1(Q_{lK})} \leq c \|v_\Gamma - \hat{v}\|_{H^{1/2}(\Gamma)},$$

where the constant c is proportional to $\max\{1\ ,\ h_A \|D_{(y_1,y_2)} \Phi\|_{L^\infty(Y)}\}$.

Proof. For the sake of simplicity we assume here $Y = [0,1]^2$.
In a *first step*, we consider the domain $U = Y \times [0, K]$ and the transformation

$$\Psi \colon Q_{lK} \to U \colon (y_1, y_2, y_3)^\top \mapsto (y_1, y_2, y_3 - h_A \Phi(y_1, y_2))^\top.$$

We intend to prove that there exists a function $\bar{w} \in [H^1_{\mathrm{per}}(U)]^3$ such that $\bar{w}|_{y_3=0} = v_\Gamma - \hat{v}$ and $\bar{w}|_{y_3=K} = 0$. Therefore, we consider the equation

$$\Delta \bar{w} = 0 \tag{14}$$

on U with the boundary conditions

$$\begin{aligned} &\bar{w} = 0 \quad \text{for } y_3 = K, \\ &\bar{w} = v_\Gamma - \hat{v} \quad \text{for } y_3 = 0, \\ &\bar{w} \text{ is } Y-\text{periodic for } (y_1, y_2) \in \partial Y. \end{aligned}$$

Since $v_\Gamma \in H^{1/2}_{\mathrm{per}}(\Gamma)$, we may expand $v_\Gamma - \hat{v}$ into a Fourier series

$$(v_\Gamma - \hat{v})(y_1, y_2) = \sum_{k,l \in \mathbb{Z}} c_{kl}\, e^{2\pi i (k y_1 + l y_2)},$$

where the coefficients c_{kl} satisfy

$$\sum_{k,l\in\mathbb{Z}} |c_{kl}|^2 (1+k^2+l^2)^{1/2} < \infty. \tag{15}$$

The function $\bar{w}$ to be constructed can be represented by a Fourier series in terms of $(y_1, y_2) \in Y$,

$$\bar{w}(y) = \sum_{k,l\in\mathbb{Z}} b_{kl}(y_3)\ e^{2\pi i(ky_1+ly_2)}.$$

Then $\bar{w}$ is a solution of (14), if the coefficients b_{kl} solve the ordinary differential equation

$$b''_{kl}(y_3) = (2\pi)^2(k^2+l^2) b_{kl}(y_3)$$

with boundary conditions

$$b_{kl}(0) = c_{kl},$$
$$b_{kl}(K) = 0.$$

Hence

$$b_{kl}(y_3) = \alpha_1\ e^{2\pi\sqrt{k^2+l^2}y_3} + \alpha_2\ e^{-2\pi\sqrt{k^2+l^2}y_3},$$

where

$$\alpha_1 = \frac{c_{kl}}{1-e^{4\pi\sqrt{k^2+l^2}K}}, \quad \alpha_2 = \frac{c_{kl}}{1-e^{-4\pi\sqrt{k^2+l^2}K}}.$$

The condition $\bar{w} \in H^1(U)$ is equivalent to

$$\sum_{k,l\in\mathbb{Z}} \|b_{kl}\|^2_{L^2(0,K)}(1+k^2+l^2) < \infty \quad \text{and} \quad \sum_{k,l\in\mathbb{Z}} \|b'_{kl}\|^2_{L^2(0,K)} < \infty$$

This can be verified by basic calculations using (15). Such a calculation also leads to the estimate

$$\|\bar{w}\|_{H^1(U)} \le c\|v_\Gamma - \hat{v}\|_{H^{1/2}(\Gamma)}.$$

The Y-periodicity of $\bar{w}$ follows immediately from its definition.

In a *second step*, we define

$$w(y) = \bar{w}(\Psi(y)) = \bar{w}(y_1, y_2, y_3 - h(y_1, y_2)),$$

where $h(y_1, y_2) := h_A\Phi(y_1, y_2)$, and prove that $w \in H^1_{\text{per}}(Q_{lK})$. Note that Φ is supposed to be a Lipschitz function. Thus the chain rule

$$Dw = (D\bar{w} \circ \Psi)D\Psi$$

is valid almost everywhere in Q_{lK}, which proves $w \in H^1_{\text{per}}(Q_{lK})$. We also get

$$\int_Y \int_{h(y_1,y_2)}^{h(y_1,y_2)+K} |w(y_1,y_2,y_3)|^2\ \mathrm{d}y_3\ \mathrm{d}(y_1,y_2) = \int_Y \int_0^K |\bar{w}(y_1,y_2,y_3)|^2\ \mathrm{d}y_3\ \mathrm{d}(y_1,y_2)$$

and thus

$$\|w\|_{L^2(Q_{lK})} = \|\bar{w}\|_{L^2(U)},$$
$$\|Dw\|_{L^2(Q_{lK})} \le C\|D\bar{w}\|_{L^2(U)}.$$

The constant in the second equation is given by $C = \max\{1\ ,\ h_A\|D_{(y_1,y_2)}\Phi\|_{L^\infty(Y)}\}$.

The *third and last step* is the proof of the existence of a divergence free function in $H^1_{\mathrm{per}}(Q_{lK})$ with the required boundary values. From the construction of $\hat{v}$ and the periodicity of w it follows

$$\int_{Q_{lK}} \operatorname{div} w \, \mathrm{d}x = \int_{\partial Q_{lK}} w \cdot n \, \mathrm{d}s = 0.$$

We follow the ideas of [14], Ch.I, §2.2 and decompose the space $[H^1_0(Q_{lK})]^3$ into the direct sum

$$[H^1_0(Q_{lK})]^3 = \{v \in [H^1_0(Q_{lK})]^3 \mid \operatorname{div} v = 0\} \oplus \{v \in [H^1_0(Q_{lK})]^3 \mid \operatorname{div} v = 0\}^\perp.$$

The exponent $\perp$ here denotes the orthogonal complement in $[H^1_0(Q_{lK})]^3$ with respect to the scalar product

$$\langle a, b\rangle = \int_{Q_{lK}} \nabla a(y) : \nabla b(y) \, \mathrm{d}y.$$

Corollary 2.4. in [14] implies the existence of a function $v \in \{v \in [H^1_0(Q_{lK})]^3 \mid \operatorname{div} v = 0\}^\perp$ with

$$\operatorname{div} v = \operatorname{div} w$$

and

$$\|\nabla v\|_{L^2(Q_{lK})} \leq c\|\operatorname{div} w\|_{L^2(Q_{lK})}.$$

Let

$$u = w - v.$$

Since $[H^1_0(Q_{lK})]^3 \subset [H^1_{\mathrm{per}}(Q_{lK})]^3$ we find

$$u \in [H^1_{\mathrm{per}}(Q_{lK})]^3$$

This is the required function. The previous results imply

$$\|u\|_{H^1(Q_{lK})} \leq c\|v_\Gamma - \hat{v}\|_{H^{1/2}(\Gamma)},$$

where the constant c is proportional to $\max\{1\ ,\ h_A\|D_{(y_1,y_2)}\Phi\|_{L^\infty(Y)}\}$. □

We extend u to Q_l by setting $u(y) = 0$ for $y \in Q_l \setminus Q_{lK}$. Obviously, $u \in [H^1_{\mathrm{per}}(Q_l)]^3$ with $\operatorname{div} u = 0$.

We return to the Stokes problem (4), (11), (12). For the function $z := v - \hat{v} - \tilde{v} - u$ we consider the problem

$$\begin{aligned} \operatorname{div} z &= 0, \\ -\eta\Delta z + \nabla p &= \eta\Delta u, \\ z &= 0 \quad \text{on } \Gamma, \\ \lim_{y_3\to\infty} z &= 0, \\ z &\text{ is } Y-\text{periodic}. \end{aligned} \tag{16}$$

If z solves (16), then v is a solution of the original problem. In order to derive a weak formulation for this problem, we assume for the moment that all functions belong to the following class

$$\mathcal{V} := \{z|_{Q_l} \mid z \in [C_0^\infty(\mathbb{R}^3)]^3,\ z|_\Gamma = 0,\ z \text{ is } Y-\text{periodic},\ \operatorname{div} z = 0\}.$$

The property $\operatorname{div} z = 0$ implies the identity

$$\Delta z = \operatorname{div}\left(\nabla z + (\nabla z)^\top\right).$$

Thus, the second equation of (16) is equivalent to

$$-\eta \operatorname{div}\left(\nabla z + (\nabla z)^\top\right) + \nabla p = \eta \operatorname{div}\left(\nabla u + (\nabla u)^\top\right). \tag{17}$$

Let w be a Y-periodic test function with $\operatorname{div} w = 0$ and $w = 0$ on Γ. Taking the scalar product of w with the previous equation and integrating over Q_l we find

$$\begin{aligned}
&\int_{Q_l} \left(-\eta \operatorname{div}\left(\nabla z + (\nabla z)^\top\right) + \nabla p\right) \cdot w \, \mathrm{d}y = \\
&\quad = \int_{Q_l} \eta \left(\nabla z + (\nabla z)^\top\right) : \nabla w - p \underbrace{\operatorname{div} w}_{=0} \, \mathrm{d}y \\
&\quad = \int_{Q_l} \frac{\eta}{2} \left(\nabla z + (\nabla z)^\top\right) : \left(\nabla w + (\nabla w)^\top\right) \, \mathrm{d}y \\
&\quad \overset{!}{=} \int_{Q_l} \eta \operatorname{div}\left(\nabla u + (\nabla u)^\top\right) \cdot w \, \mathrm{d}y \\
&\quad = -\int_{Q_l} \frac{\eta}{2} \left(\nabla u + (\nabla u)^\top\right) : \left(\nabla w + (\nabla w)^\top\right) \, \mathrm{d}y
\end{aligned}$$

Let

$$\begin{aligned}
a(z, w) &:= \int_{Q_l} \frac{\eta}{2} \left(\nabla z + (\nabla z)^\top\right) : \left(\nabla w + (\nabla w)^\top\right) \, \mathrm{d}y, \\
\ell(w) &:= -\int_{Q_l} \frac{\eta}{2} \left(\nabla u + (\nabla u)^\top\right) : \left(\nabla w + (\nabla w)^\top\right) \, \mathrm{d}y.
\end{aligned}$$

In order to prove the existence of solutions for a weak formulation of our problem we intend to apply the Lax-Milgram Theorem. Therefore, it is necessary to prove that the bilinear form a is continuous and elliptic with respect to a suitable norm on $\mathcal{V}$. Here, we will not choose the norm of $H^1(Q_l)$ since we can neither prove the Second Korn inequality nor the Poincare inequality which would imply the ellipticity of a with respect to the H^1-norm. Instead, we consider the H^1-seminorm

$$\|z\|_V := \left(\int_{Q_l} |\nabla z(y)|^2 \, \mathrm{d}y\right)^{1/2},$$

which is a norm on $\mathcal{V}$ due the condition $z|_\Gamma = 0$. Le V be the closure of $\mathcal{V}$ with respect to this norm. Then V is a Hilbert space with scalar product

$$(z_1, z_2)_V = \int_{Q_l} \nabla z_1(y) : \nabla z_2(y) \, \mathrm{d}y.$$

Note that V might not be equal to the closure of $\mathcal{V}$ with respect to the H^1-norm. Obviously, we have the inclusion

$$\overline{\mathcal{V}}^{\|\cdot\|_{H^1(Q_l)}} \subset V$$

with continuous imbedding. The weak formulation of the problem is given by

Find $z \in V$ such that

$$a(z, w) = \ell(w) \tag{18}$$

for all $w \in V$.

The following theorem guaranties that this problem has a unique solution:

Theorem 3.2. *Assume that Γ is Lipschitz continuous, i.e. Φ is Lipschitz continuous, and that $v_\Gamma \in H^{1/2}(\Gamma)$. Then (18) has a unique solution $z \in V$. Furthermore, there exists a $p \in L^2_{\text{loc}}(Q_l)$ that is uniquely defined up to a constant such that*

$$-\eta \Delta z + \nabla p = \eta \Delta u$$

in the distribution sense in Q_l. Moreover,

$$\|z\|_V \le c\|v_\Gamma - \hat{v}\|_{H^{1/2}(\Gamma)},$$

where the constant c is proportional to $\max\{1\ ,\ h_A\|D_{(y_1,y_2)}\Phi\|_{L^\infty(Y)}\}$.

Before we prove this theorem we refer classical results which can be found e.g. in [14], Chapter I, §2, and [23], Chapter I, §1:

Proposition 3.3. *Let $\Omega \subset \mathbb{R}^N$ be an open set.*

i) If $f = (f_1, \dots, f_N)$, where $f_i \in \mathcal{D}'(\Omega)$ is a distribution on Ω for $i = 1, \dots, N$, then a necessary and sufficient condition for

$$f = \operatorname{grad} p$$

with some distribution $p \in \mathcal{D}'(\Omega)$ is

$$\langle f, \nu\rangle = 0 \quad \text{for all } \nu \in \{\nu \in C_0^\infty(\Omega) \mid \operatorname{div}\nu = 0\}.$$

ii) If a distribution $p \in \mathcal{D}'(\Omega)$ has all its first derivatives $D_i p$, $i = 1, \dots, N$, in $H^{-1}(\Omega)$, then $p \in L^2_{\text{loc}}(\Omega)$.

iii) Let Ω be a connected and bounded open set with Lipschitz-boundary. If

$$p \in L^2_{\text{loc}}(\Omega) \quad \text{and} \quad \operatorname{grad} p \in H^{-1}(\Omega),$$

then $p \in L^2(\Omega)$.

We also need a version of the First Korn inequality:

Theorem 3.4. *Let $\Omega = Y \times \mathbb{R}$ with $Y = [0,1]^2$ and let*

$$\mathcal{W} = \{w|_\Omega \mid w \in [C_0^\infty(\mathbb{R}^3)]^3,\ w(y_1, y_2, 0) = 0,\ w \text{ is } Y-\text{periodic}\}.$$

Let W be the closure of $\mathcal{W}$ with respect to the H^1-norm or the H^1-seminorm. Then, for all $u \in W$ the following inequality holds:

$$\|\nabla u\|^2_{L^2(\Omega)} \le 2\|e(u)\|^2_{L^2(\Omega)}.$$

Proof. For the proof we use ideas used in [15], Chapter 2.5, Lemma 5.2. Let $\hat{u}$ be the Fourier transform of u with respect to y_3,

$$\hat{u}(y_1, y_2, \xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} u(y_1, y_2, y_3) e^{-i\xi y_3}\ \mathrm{d}y_3.$$

The Fourier transform is a unitary transform,

$$\int_{\mathbb{R}} u(y_1, y_2, y_3)\overline{v(y_1, y_2, y_3)}\ \mathrm{d}y_3 = \int_{\mathbb{R}} \hat{u}(y_1, y_2, \xi)\overline{\hat{v}(y_1, y_2, \xi)}\ \mathrm{d}\xi$$

and in particular

$$\int_{\mathbb{R}} |u(y_1, y_2, y_3)|^2\ \mathrm{d}y_3 = \int_{\mathbb{R}} |\hat{u}(y_1, y_2, \xi)|^2\ \mathrm{d}\xi$$

holds. We expand $\hat{u}$ into a Fourier series with respect to y_1 and y_2: For $k = 1, 2, 3$ we have

$$\hat{u}_k(y_1, y_2, \xi) = \sum_{m,n=-\infty}^{\infty} c_{kmn} e^{2\pi i(my_1 + ny_2)}$$

with coefficients c_{kmn} given by

$$c_{kmn} = \int_Y \hat{u}_k(y_1, y_2, \xi) e^{-2\pi i(my_1 + ny_2)}\ \mathrm{d}y_1 \mathrm{d}y_2.$$

Parseval's equality yields

$$\int_Y |\hat{u}_k(y_1, y_2, \xi)|^2 \, \mathrm{d}y_1 \mathrm{d}y_2 = \sum_{m,n=-\infty}^{\infty} |c_{kmn}|^2.$$

From this representation we find

$$\begin{aligned}
\|e(u)\|^2_{L^2(\Omega)} &= \int_\Omega \Big[(\partial_1 u_1)^2 + (\partial_2 u_2)^2 + (\partial_3 u_3)^2 \\
&\quad + \tfrac{1}{2}(\partial_1 u_2 + \partial_2 u_1)^2 + \tfrac{1}{2}(\partial_1 u_3 + \partial_3 u_1)^2 + \tfrac{1}{2}(\partial_3 u_2 + \partial_2 u_3)^2 \Big] \, \mathrm{d}y \\
&= \int_{\mathbb{R}} \sum_{m,n=-\infty}^{\infty} \Big[4\pi^2 m^2 |c_{1mn}|^2 + 4\pi^2 n^2 |c_{2mn}|^2 + \xi^2 |c_{3mn}|^2 \\
&\quad + 2\pi^2 m^2 |c_{2mn}|^2 + 2\pi^2 n^2 |c_{1mn}|^2 + 2\pi^2 m^2 |c_{3mn}|^2 + 2\pi^2 n^2 |c_{3mn}|^2 \\
&\quad + \tfrac{1}{2}\xi^2 |c_{1mn}|^2 + \tfrac{1}{2}\xi^2 |c_{2mn}|^2 + 4\pi^2 mn \, \mathrm{Re}(c_{1mn}\overline{c_{2mn}}) \\
&\quad + 2\pi m \, \mathrm{Re}(i\xi c_{1mn}\overline{c_{3mn}}) + 2\pi n \, \mathrm{Re}(i\xi c_{2mn}\overline{c_{3mn}}) \Big] \, \mathrm{d}\xi \\
&= \frac{1}{2}\|\nabla u\|^2_{L^2(\Omega)} + \int_{\mathbb{R}} \sum_{m,n=-\infty}^{\infty} \Big[2\pi^2 m^2 |c_{1mn}|^2 + 2\pi^2 n^2 |c_{2mn}|^2 \\
&\quad + \tfrac{1}{2}\xi^2 |c_{3mn}|^2 + 4\pi^2 mn \, \mathrm{Re}(c_{1mn}\overline{c_{2mn}}) + 2\pi m \, \mathrm{Re}(i\xi c_{1mn}\overline{c_{3mn}}) \\
&\quad + 2\pi n \, \mathrm{Re}(i\xi c_{2mn}\overline{c_{3mn}}) \Big] \, \mathrm{d}\xi \\
&\geq \frac{1}{2}\|\nabla u\|^2_{L^2(\Omega)},
\end{aligned}$$

since

$$\frac{1}{2}|z_1 + z_2 + z_3|^2 \geq 0,$$

with

$$\begin{aligned}
z_1 &= 2\pi m \; c_{1mn}, \\
z_2 &= 2\pi n \; c_{2mn}, \\
z_3 &= i\xi \; c_{3mn}.
\end{aligned}$$

Note that we changed the order of differentiation and the infinte sum of the Fourier series in the above calculations. This can be done for continuously differentiable Y-periodic functions, see e.g. [16], chapter 2.4. Since these functions are dense in the space W, the result can be extended to our case. □

Now we prove Theorem 3.2:

Proof of Theorem 3.2. In order to apply the Lax-Milgram Theorem it is necessary to prove that the bilinear form a is V-elliptic and continuous. The Lax-Milgram Theorem then implies that (18) has a unique solution and that

$$\|z\|_V \leq c\|\ell\|_{V'}.$$

Continuity:

Young's inequality

$$2ab \leq a^2 + b^2, \quad \forall a, b \in \mathbb{R},$$

implies

$$\|e(z)\|^2_{L^2(Q_l)} \leq \|\nabla z\|^2_{L^2(Q_l)}$$

for all $z \in V$, where $e(z) = \frac{1}{2}\left(\nabla z + (\nabla z)^\top\right)$. This yields the continuity of a:

$$|a(z,w)| \leq 2\eta \|e(z)\|_{L^2(Q_l)} \, \|e(w)\|_{L^2(Q_l)} \leq 2\eta \|z\|_V \, \|w\|_V .$$

V-ellipticity:
First we extend z to the strip $Y \times \mathbb{R}$ by setting

$$z(y) = \begin{cases} z(y_1, y_2, y_3), & y_3 \geq h_A \Phi(t, x, y_1, y_2), \\ 0, & y_3 < h_A \Phi(t, x, y_1, y_2), \end{cases}$$

The extended function z belongs to the space W defined in Theorem 3.4 and we have

$$\|z\|_W = \|z\|_V$$

and

$$\|e(z)\|_{L^2(Y \times \mathbb{R})} = \|e(z)\|_{L^2(Q_l)}.$$

Thanks to these equalities and Theorem 3.4 Korn's first inequality is true, that is

$$\|\nabla z\|^2_{L^2(Q_l)} \leq 2\|e(z)\|^2_{L^2(Q_l)}.$$

Hence a is V-elliptic.
Existence of p:
For the solution z of (18) the mapping $a(z,\cdot) - \ell(\cdot)$ belongs to the space $[H^{-1}(Q_l)]^3$ with

$$a(z,\nu) - \ell(\nu) = 0, \quad \forall \nu \in \mathcal{V}.$$

Since $\{\nu \in C_0^\infty(Q_l) \,|\, \operatorname{div} \nu = 0\} \subset \mathcal{V}$ holds, Proposition 3.3 implies that there exists a $p \in L^2_{\text{loc}}(Q_l)$ such that

$$-\eta \Delta z + \nabla p = \eta \Delta u$$

in the distributional sense in Q_l. □

The solution (v, p) of the Stokes problem is needed as a boundary condition for the elasticity equation. This condition is given on Γ by

$$-\sigma(u)n + \eta\left(\nabla v + (\nabla v)^\top\right)n - pn = 0,$$

where u is the mechanical displacement field and n the outer normal on Q_l and Γ. Therefore the expression

$$\left(\eta\left(\nabla v + (\nabla v)^\top\right) - p\mathbf{I}\right)n$$

should be well defined on Γ in a certain sense. Let Q_{lK} be the domain defined above which is bounded with a Lipschitz boundary. The previous results imply that the restrictions of v and p to Q_{lK} belong to $[H^1(Q_{lK})]^3$ and $L^2(Q_{lK})$, respectively. Due to

$$\eta \Delta v + \operatorname{grad} p = \operatorname{div}\left(\eta\left(\nabla v + (\nabla v)^\top\right) + p\mathbf{I}\right) = 0 \in L^2(Q_{lK}),$$

we conclude

$$\left(\eta\left(\nabla v + (\nabla v)^\top\right) - p\mathbf{I}\right)n \in H^{-1/2}(\Gamma).$$

4 The elasticity equation

In this section, we consider the elasticity equation (5) with boundary conditions (6), (13) and periodic boundary conditions for $(y_1, y_2) \in \partial Y$. The upper boundary of Q_s is given by Γ and the lower boundary by

$$\bar{\Gamma} = \{y \in \mathbb{R}^3 | (y_1, y_2) \in Y, y_3 = 0\}.$$

For the boundary condition $u = b$ on $\bar{\Gamma}$ we assume $b \in H^{1/2}_{\text{per}}(\bar{\Gamma})$. By the technique used in the proof of Lemma 3.1 we find that there is a Y-periodic function $\hat{u}$ in $\in H^1_{\text{per}}(Q_s)$ with $\hat{u}|_{\hat{\Gamma}} = b$. Inserting $z = u - \hat{u}$ in (5), we get

$$-\operatorname{div}\sigma(z) = \operatorname{div}\sigma(\hat{u}), \quad \text{in } Q_s \tag{19}$$

with boundary conditions

$$\begin{aligned} \sigma(z)n &= g - \sigma(\hat{u})n \quad \text{on } \Gamma, \\ z &= 0 \quad \text{on } \bar{\Gamma}, \\ z &\text{ is } Y-\text{periodic for } (y_1, y_2) \in \partial Y, \end{aligned} \tag{20}$$

where

$$g = \eta\left(\nabla v + (\nabla v)^\top\right) n - pn.$$

Let us assume for the moment that all functions are smooth. Let w be Y-periodic with $w|_{\bar{\Gamma}} = 0$. We take the scalar product of (19) with w and integrate over Ω:

$$\begin{aligned} \int_{Q_s} -(\operatorname{div}\sigma(z)) \cdot w \, \mathrm{d}y &= \int_{Q_s} \sigma(z) : \nabla w \, \mathrm{d}y - \int_{\partial Q_s} \sigma(z)n \cdot w \, \mathrm{d}a \\ &= \int_{Q_s} \sigma(z) : \nabla w \, \mathrm{d}y - \int_{\Gamma} \sigma(z)n \cdot w \, \mathrm{d}a \\ &\overset{!}{=} \int_{Q_s} (\operatorname{div}\sigma(\hat{u})) \cdot w \, \mathrm{d}y \\ &= -\int_{Q_s} \sigma(\hat{u}) : \nabla w \, \mathrm{d}y + \int_{\Gamma} \sigma(\hat{u})n \cdot w \, \mathrm{d}a. \end{aligned}$$

Using the boundary conditions we get

$$\begin{aligned} a(z, w) &:= \int_{Q_s} \sigma(z) : \nabla w \, \mathrm{d}y \\ &= -\int_{Q_s} \sigma(\hat{u}) : \nabla w \, \mathrm{d}y + \langle g, w \rangle_{H^{-1/2}(\Gamma), H^{1/2}(\Gamma)} =: \ell(w). \end{aligned} \tag{21}$$

We introduce the space of test functions

$$V = \{v \in H^1(Q_s) \mid v|_{\bar{\Gamma}} = 0, v \text{ is } Y-\text{periodic}\}$$

and state the weak formulation of the problem:

Find $z \in V$ such that

$$a(z, w) = \ell(w), \tag{22}$$

for all $w \in V$.

The following theorem guarantiees that this problem has a unique solution:

Theorem 4.1. *Assume that ∂Q_s is a Lipschitz boundary, i.e. Φ is Lipschitz. Let $b \in H^{1/2}_{\text{per}}(\bar{\Gamma})$. Then (22) has a unique solution $z \in V$. Moreover,*

$$\|z\|_V \le C\left(\|b\|_{H^{1/2}(\bar{\Gamma})} + \|g\|_{H^{-1/2}(\Gamma)}\right).$$

Proof. The bilinear form a is V-elliptic due to Korn's inequality (see e.g. [20], Thm. 2.7., p21) and continuous due to Young's and Cauchy-Schwarz' inequality. The Lax-Milgram Theorem yields the result. □

5 The microscopic phase field equations

In this section we discuss the solvability of the phase field version of the microscopic BCF-model (7) and (8). This system is solved for the phase field Φ and the surface concentration c^S; f is a multi-well potential with minima at integer values, e.g. $f(\Phi) = -\cos(2\pi\Phi)$, and q is given by (9). These equations are valid for every $x \in S_0$ in $I \times Y$, where $I = [0,T]$ is a time intervall and Y a periodicity cell. Furthermore we have the initial conditions

$$c^S(0,x,y) = c^{S0}(x,y), \tag{23}$$

$$\Phi(0,x,y) = \Phi^0(x,y), \tag{24}$$

and periodic boundary conditions for in $(y_1,y_2) \in Y$. We consider test functions $w_1, w_2 \in L^2(I; H^1_{\text{per}}(Y))$, multiply equations (7) and (8) with w_1 and w_2 respectively, integrate by parts and get the following weak formulation of the problem:

Find c^S, $\Phi \in L^2(I; H^1_{\text{per}}(Y))$ with $\partial_t c^S$, $\partial_t \Phi \in L^2(I; H^1_{\text{per}}(Y)')$ such that the initial conditions (23) and (24) are satisfied and for every $w_1, w_2 \in L^2(I; H^1_{\text{per}}(Y))$ the following equations are true:

$$\int_I \left(\langle \partial_t c^S, w_1 \rangle + \varrho_s h_A \langle \partial_t \Phi, w_1 \rangle + \int_Y \left(D_s \nabla c^S \cdot \nabla w_1 + \left(\tfrac{c^S}{\tau_S} - \tfrac{c^V}{\tau_V} \right) w_1 \right) \mathrm{d}y \right) \mathrm{d}t = 0, \tag{25}$$

$$\int_I \left(\alpha \xi^2 \langle \partial_t \Phi, w_2 \rangle + \int_Y \left(\xi^2 \, \nabla \Phi \cdot \nabla w_2 + \left(f'(\Phi) + q(c^S, u, \Phi) \right) w_2 \right) \mathrm{d}y \right) \mathrm{d}t = 0. \tag{26}$$

Here, $\langle \cdot, \cdot \rangle$ denotes the dual pairing in $H^1_{\text{per}}(Y)$. These equations have the same structure as the microscopic problem in [8]. We get the same existence result:

Theorem 5.1. *Let be $c^{S0} \in L^2(Y)$, $\Phi^0 \in H^1(Y)$. Furthermore, suppose that f' and q have at most linear growth with respect to c^S and Φ and that the constants D_S, α, ξ, h_A, ϱ_S, τ_V and τ_S are positive. Then, the microscopic problem (25) and (26) at a fixed point $x \in S_0$ with given $c^V = c^V(\cdot, x) \in L^2(I)$ has a unique solution.*

Proof. We refer to [8], where these results are proven for a very similar problem. □

As mentioned in Sections 3 and 4 we need a higher regularity for Φ than it is given in the previous theorem, namely the Lipschitz continuity of Φ with respect to y, which is equivalent to $\Phi(t,x,\cdot) \in W^1_\infty(Y)$. We adapt the methods of [9], Chapters 2 and 3, to prove that this is true. Before we do that, we state a regularity result that we need for the proof:

Theorem 5.2. *Suppose $\Omega \subset \mathbb{R}^N$ is a domain with C^2-smooth boundary $\partial\Omega$, $I = [0,T]$, $r > 1$ and $r \neq \frac{3}{2}$. Consider the heat equation*

$$\partial_t w - d\Delta w = g$$

with $d > 0$ on $I \times \Omega$ with boundary condition $w = 0$ on $I \times \partial\Omega$ and initial condition $w(\cdot, 0) = w_0$ in Ω. Suppose $g \in L^r(I \times \Omega)$ and $w_0 \in W_r^{2-2/r}(\Omega)$. Then the solution w of this problem is an element of the space $W_r^{1,2}(I \times \Omega)$, where the first upper index denotes the time reguilarity and the second one the space regularity. Furthermore, w satisfies

$$\|w\|_{W_r^{1,2}(I\times\Omega)} \leq C \left(\|g\|_{L^r(I\times\Omega)} + \|w_0\|_{W_r^{2-2/r}(\Omega)} \right),$$

with a constant C independent of f and w_0.

This theorem is a special case of Theorem 9.1 in Chapter IV of [17]. With the help of this theorem we can prove the following statement:

Theorem 5.3. *Suppose $c^{S0} \in W^{2-2/s}_{s,\mathrm{per}}(Y)$, $\Phi^0 \in W^{2-2/s}_{s,\mathrm{per}}(Y)$ and $c^V(\cdot,x) \in L^s(I)$ for a $s > 4$. Furthermore, let $f(\Phi) = -\cos(2\pi\Phi)$. Then, the solution (Φ, c^S) of the microscopic problem (25) and (26) satisfies $\Phi \in L^\infty(I, W^1_\infty(Y))$ and $c^S \in L^\infty(I, W^1_\infty(Y))$ and the estimate*

$$\begin{aligned}\|\Phi\|_{L^\infty(I,W^1_\infty(Y))} + \|c^S\|_{L^\infty(I,W^1_\infty(Y))} \le C\big(1 &+ \|c^S\|_{L^2(I,H^1(Y))} + \|\Phi\|_{L^2(I,H^1(Y))}\\ &+ \|\partial_t\Phi\|_{L^2(I\times Y)} + \|c^V(\cdot,x)\|_{L^s(I)}\\ &+ \|\Phi^0\|_{W^{s-2/s}_s(Y)} + \|c^{S0}\|_{W^{2-2/s}_s(Y)}\big)\end{aligned}$$

is valid. The constant C depends on u, but is independent of Φ, c^S, Φ^0 and c^{S0}.

Proof. Let Ω be a bounded domain such that $\bar{Y} \subset \Omega$ with C^2–smooth boundary $\partial\Omega$. Let $\chi \in C_0^\infty(\Omega)$ be a cut–off function with $\chi|_Y = 1$ and $0 \le \chi(y) \le 1$ for all $y \in \Omega$. The functions Φ and c^S are Y-periodic in $H^1(Y)$ which implies that they can be extended periodically to Ω with $\Phi, c^S \in H^1(\Omega)$. In the following we consider the functions $\chi\Phi$ and χc^S. If Φ and c^S solve (25) and (26) on $I \times Y$, then $\chi\Phi$ and χc^S solve

$$\alpha\xi^2\partial_t(\chi\Phi) - \xi^2\Delta(\chi\Phi) = -\chi\left(f'(\Phi) + q(c^S,u,\Phi)\right) - \xi^2\left(\Phi\Delta\chi + 2\nabla\chi\nabla\Phi\right), \tag{27}$$

$$\partial_t(\chi c^S) - D_S\Delta(\chi c^S) = \chi\left(\frac{c^V}{\tau_V} - \frac{c^S}{\tau_S} - \varrho_S h_A \partial_t\Phi\right) - D_S\left(c^S\Delta\chi + 2\nabla\chi\nabla c^S\right) \tag{28}$$

on $I \times \Omega$ with homogeneous Dirichlet conditions on $I \times \partial\Omega$ and initial conditions

$$\begin{aligned}\chi c^S(0,x,y) &= \chi c^{S0}(x,y),\\ \chi\Phi(0,x,y) &= \chi\Phi^0(x,y).\end{aligned}$$

Let us have a look at the regularity of the right hand sides of these equations. We start with (27): From $f'(\Phi) \in L^\infty(I \times \Omega)$, $\Phi \in L^2(I, H^1(\Omega))$, $\nabla\Phi \in L^2(I \times \Omega)$ and $q \in L^2(I, H^1(\Omega))$ the application of Theorem 5.2 yields

$$\chi\Phi \in W^{1,2}_2(I \times \Omega)$$

and therefore

$$\Phi \in W^{1,2}_2(I \times Y).$$

The embedding $W^{1,2}_2(I \times Y) \hookrightarrow W^{0,1}_4(I \times Y)$ then gives us

$$\Phi \in W^{0,1}_4(I \times Y),$$

with

$$\|\Phi\|_{W^{0,1}_4(I\times Y)} \le C\left(1 + \|c^S\|_{L^2(I,H^1(Y))} + \|\Phi\|_{L^2(I,H^1(Y))} + \|\Phi^0\|_{W^{2-2/s}_s(Y)}\right).$$

This implies $\partial_t\Phi \in L^2(I \times Y)$ and, with $c^V(\cdot,x) \in L^s(I)$ and $c^S \in L^2(I, H^1(Y))$, Theorem 5.2 applied to equation (28) yields

$$c^S \in W^{1,2}_2(I \times Y),$$

and thus

$$c^S \in W^{0,1}_4(I \times Y)$$

with

$$\|c^S\|_{W^{0,1}_4(I\times Y)} \le C\left(\|c^V(\cdot,x)\|_{L^2(I)} + \|\partial_t\Phi\|_{L^2(I\times Y)} + \|c^S\|_{L^2(I,H^1(Y))} + \|c^{S0}\|_{H^1(Y)}\right).$$

We repeat the same argument for both equations with 4 as the order of integration instead of 2 which gives us

$$\begin{aligned}\Phi &\in W^{1,2}_4(I \times Y),\\ c^S &\in W^{1,2}_4(I \times Y),\end{aligned}$$

and thus

$$\Phi \in W_s^{0,1}(I \times Y),$$
$$c^S \in W_s^{0,1}(I \times Y),$$

for all $s \geq 1$. Another repetition of this procedure yields

$$\Phi \in W_s^{1,2}(I \times Y),$$
$$c^S \in W_s^{1,2}(I \times Y)$$

for any $s < +\infty$. Next, for $0 < \lambda < 1$ we have the interpolation

$$W_s^{1,2}(I \times Y) \hookrightarrow W_s^{\lambda}(I, W_s^{2(1-\lambda)}(Y)),$$

and together with the embeddings

$$W_s^{\lambda}(I, W_s^{2(1-\lambda)}(Y)) \hookrightarrow L^{\infty}(I, W_s^{2(1-\lambda)}(Y)),$$
$$W_s^{2(1-\lambda)}(Y) \hookrightarrow W_{\infty}^{1}(Y),$$

that are valid for $s > 4$, we obtain

$$\Phi \in L^{\infty}(I, W_{\infty}^{1}(Y)),$$
$$c^S \in L^{\infty}(I, W_{\infty}^{1}(Y)),$$

and the estimate

$$\begin{aligned}\|\Phi\|_{L^{\infty}(I,W_{\infty}^{1}(Y))} + \|c^S\|_{L^{\infty}(I,W_{\infty}^{1}(Y))} \leq C\big(&1 + \|c^S\|_{L^2(I,H^1(Y))} + \|\Phi\|_{L^2(I,H^1(Y))} \\ &+ \|\partial_t \Phi\|_{L^2(I\times Y)} + \|c^V(\cdot,x)\|_{L^s(I)} \\ &+ \|\Phi^0\|_{W_s^{s-2/s}(Y)} + \|c^{S0}\|_{W_s^{2-2/s}(Y)}\big)\end{aligned}$$

where the constant C depends on u, but is independent of Φ, c^S, Φ^0 and c^{S0}. □

6 The macroscopic equations

Analogously to the model for liquid phase epitaxy without elasticity (see [8]), we notice that the Navier-Stokes equations decouples from the other equations. In the following we will consider the velocity V as given. It remains to consider the convection-diffusion equation (2) together with the coupling (10) and homogeneous Neumann conditions on $Q \setminus S_0$. This problem also occurs in the model without elasticity and its solvability was investigated in [8]. Thus, we only formulate the results here. The weak formulation of the problem is given by:

Find $c^V \in L_2(I, H^1(Q))$ with $\partial_t c^V \in L_2(I, H^1(Q)')$ such that the initial condition $c^V(0,x) = c^{V0}(x)$ is satisfied for $x \in Q$ and for every $u \in L_2(I; H^1(Q))$

$$\int_I \left(\langle \partial_t c^V, u \rangle + \int_Q (v \cdot \nabla c^V u + D_V \nabla c^V \cdot \nabla u)\, dx \right) dt = \int_{I\times S_0} m_A \left(\frac{\bar{c}^S}{\tau_S} - \frac{c^V}{\tau_V} \right) u\, ds_x\, dt, \qquad (29)$$

where $\langle \cdot, \cdot \rangle$ denotes the dual pairing in $H^1(Q)$. We get the following theorem:

Theorem 6.1. *Suppose that D_V, τ_V, τ_S and m_A are positive constants. For given $\bar{c}^S \in L^2(I \times S_0)$ and $v \in L^{\infty}(I, L^2(Q)) \cap L^2(I, H^1(Q))$, with $\operatorname{div} v = 0$ in $I \times Q$ and $v \cdot n = 0$ in $I \times \partial Q$, problem (29) has a unique solution.*

7 Summary

We considered the single parts of the two-scale model for liquid phase epitaxy with elasticity with coupling data assumed to be given. We proved that all these parts have unique solutions and that the phase field Φ is sufficiently regular to be used for the description of the boundaries of the domains for the elasticity equation and the Stokes system. We also studied the dependences of u and v on Φ.
The next step will be the analysis of the fully coupled model equations. This shall be done by a fixed point approach in order to show the solvability of the model. It remains to justify the formal derivation of the two-scale model by proving an error estimate in dependence of the scale parameter.

References

[1] G. Allaire. Homogenization and two-scale convergence. *SIAM J. Math. Anal.* **23**(6), 1482–1518, 1992.

[2] W. K. Burton, N. Cabrera, F. C. Frank. The growth of crystals and the equilibrium structure of their surfaces. *Phil. Trans. Roy. Soc.* **243**, 299–358, 1951.

[3] P. Cermelli, M. Jabbour. Multispecies epitaxial growth on vicinal surfaces with chemical reactions and diffusion. *Proc. R. Soc. A* **461**, 3483–3504, 2005.

[4] V. Chalupecky, Ch. Eck, H. Emmerich. Computation of nonlinear multiscale coupling effects in liquid phase epitaxy. *Eur. Phys. J. Special Topics* **149**, 1–17, 2007.

[5] D. Cioranescu, A. Damlamian, G. Griso. Periodic unfolding and homogenization. *C. R. Math. Acad. Sci. Paris* **335**(1), 99–104, 2002.

[6] D. Cioranescu, A. Damlamian, G. Griso. The periodic unfolding method in homogenization. *SIAM J. Math. Anal.* **40**(4), 1585–1620, 2008.

[7] D. Cioranescu, P. Donato. *An introduction to homogenization.* Oxford Lecture Series in Mathematics and its Applications, Oxford University Press Inc., New York, 1999.

[8] Ch. Eck, H. Emmerich. A two-scale model for liquid-phase epitaxy. *Math. Methods Appl. Sci.* **32**(1), 12–40, 2009.

[9] Ch. Eck. A Two-Scale Phase Field Model for Liquid–Solid Phase Transitions of Binary Mixtures with Dendritic Microstrucure. *Habilitationsschrift*, Universität Erlangen-Nürnberg, 2004.

[10] Ch. Eck, H. Emmerich. Liquid-phase epitaxy with elasticity. *Preprint 197*, DFG SPP 1095, 2006.

[11] Ch. Eck. Homogenization of a phase field model for binary mixtures. *Multiscale Model. Simul.* **3**(1), 1–27, 2004.

[12] Ch. Eck. Analysis of a two-scale phase field model for liquid-solid phase transitions with equiaxed dendritic microstructures. *Multiscale Modeling and Simulation* **3**(1), 28–49, 2004.

[13] H. Emmerich. Modeling elastic effects in epitaxial growth *Continuum Mech. Thermodyn.* **15**, 197–215, 2003.

[14] V. Girault, P.-A. Raviart. *Finite Element Methods for Navier-Stokes Equations, Theory and Algorithms.* Springer-Verlag, 1986.

[15] I. Hlaváček, J. Haslinger, J. Nečas, J. Lovišek. *Solution of Variational Inequalities in Mechanics.* Springer-Verlag, 1988.

[16] A. Kufner, J. Kadlec. *Fourier Series.* Iliffe Books, Butterworth, 1971.

[17] O.A. Ladyženskaja, V.A. Solonnikov, N.N. Ural'ceva. *Linear and Quasi-linear Equations of Parabolic Type*. MS Transl. of Math. Monographs Vol. 23, Providence, Rhode Island, 1968.

[18] T. S. Lo, R. V. Kohn. A new approach to the continuum modeling of epitaxial growth: slope selection, coarsening, and the role of uphill current. *Physica D* **161**, 237–257, 2002.

[19] G. Nguetseng. A general convergence result for a functional related to the theory of homogenization. *SIAM J. Math. Anal.* **20**(3), 608–623, 1989.

[20] O.A. Oleinik, A.S. Shamaev, G.A. Yosifian. *Mathematical Problems in Elasticity and Homogenization.* North Holland, Elsevier Scientific Publishers, Amsterdam, 1992.

[21] F. Otto, P. Penzler, A. Rätz, T. Rump, A. Voigt. A diffuse-interface approximation for step flow in epitaxial growth. *Nonlinearity* **17**, 477–491, 2004

[22] G. Russo, P. Smereka. Computation of strained epitaxial growth in three dimensions by kinetic Monte Carlo *J. Comput. Physics* **214**, 809–828, 2006.

[23] R. Temam. *Navier-Stokes Equations*, North-Holland Publishing Company - Amsterdam · New York · Oxford, 1977.

[24] J. Villain. Continuum models of crystal-growth from atomic-beams with and without desorption. *J. Phys. I* **1**, 19–42, 1991.

[25] A. Visintin. Towards a two–scale calculus. *ESAIM: COCV* **12**, 371–397, 2006.

[26] Y. Xiang. Derivation of a continuum model for epitaxial growth with elasticity on vicinal surfaces. *SIAM J. Appl. Math.* **63**(1) 241–258, 2002.

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