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Fachbereich Mathematik
Fakultät Mathematik und Physik
Universität Stuttgart
Pfaffenwaldring 57
D-70 569 Stuttgart

E-Mail: preprints@mathematik.uni-stuttgart.de
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Contents

A Two Scale Model for Liquid Phase Epitaxy with Elasticity: An Iterative Procedure.

Christof Eck, Michael Kutter*, Anna-Margarete Sändig, Christian Rohde

Institute of Applied Analysis and Numerical Simulation,
University of Stuttgart,
Pfaffenwaldring 57, 70569 Stuttgart.

Abstract

Epitaxy is a technically relevant process since it gives the possibility to generate microstructures of different morphologies. These microstructures can be influenced by elastic effects in the epitaxial layer. We consider a two scale model including elasticity, introduced in [7]. The coupling of the microscopic and the macroscopic equations is described by an iterative procedure. We concentrate on the microscopic equations and study their solvability in appropriate function spaces. As the main results we prove the existence and uniqueness of solutions of the three single parts of the microscopic problem. The composition of the corresponding solution operators maps a suitable function space into itself. These results are a first step in the proof of existence of solutions via suitable fixed point arguments of the fully coupled two scale model.

Keywords: liquid phase epitaxy with elasticity, two scale model, iterative procedure, existence and regularity of solutions

AMS Subject Classification: 74K35, 76D03, 35K40, 35K58

1 Introduction

Epitaxy is a technical process to produce thin films and layers. During this process single molecules are deposited on the growing film where they 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. Liquid phase epitaxy (LPE) is one of several epitaxial techniques. For LPE the molecules that contribute to the growth process are dissolved in a liquid solution and transported to the layer by convection and diffusion. It is known that some microstructures that arise in LPE are generated by instabilities in the elastic deformation in the solid layer, see [10], [28] and the references therein.

There are different approaches to model epitaxial growth. The Burton–Cabrera–Frank model (BCF–model) [4], which was originally derived for molecular beam epitaxy, 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 [14], [10]: the boundaries of the mono-molecular steps are approximated by a diffuse phase boundary that is described by an additional phase field, [17]. 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 [26]. Sometimes also purely atomistic models are used in corresponding Monte–Carlo–simulations [21]; due to the huge number of needed unknowns they are, however, only applicable for very small length scales.

*EMail: `Michael.Kutter@mathematik.uni-stuttgart.de`

The direct numerical simulation of an epitaxial process for technically relevant length scales is cumbersome or even impossible because a corresponding numerical grid has to resolve the full microstructure. Homogenization techniques can be used to derive two or multi scale models which combine microscopic problems for the evolution of the microstructure and macroscopic equations for the description of processes "far away" from the interface. In [6], a two scale model for LPE is derived by homogenization via asymptotic expansion in combination with a matched asymptotic expansion close to the solid film. It describes the transport processes in the liquid solution by macroscopic Navier–Stokes–Equations and a macroscopic convection–diffusion–equation while the evolution of the microstructures is modeled by a phase field version of the BCF–model. Elastic effects in the layer are neglected.

In [7], an elastic equation was included into the model of [6]. As a consequence, the microscopic part becomes much more complicated. In addition to the phase field version of the BCF–model, a microscopic elastic equation and a microscopic Stokes system occur where the corresponding domains of both of these problems depend on the phase field. Furthermore, the domain of the Stokes system is unbounded in one direction. The macroscopic part is the same as in [6].

In this paper we consider the model of [7]. We suggest an iterative procedure and investigate the analytical solvability of each single step regarding the derivation of a fundament for a numerical scheme and the corresponding numerical analysis. We define and study the properties of corresponding solution operators and prove that the composition of these operators maps a suitable function space into itself. Thus, these results are a first step in the proof of existence of solutions of the fully coupled two scale model, as it has been done in [6] for the model without elasticity.

2 The Two Scale Model

This section introduces the two scale model, for details on its derivation see [7]. The physical situation is the following: Consider a domain $Q \subset \mathbb{R}^3$ 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 time dependent domain occupied by this film is denoted by $Q^S = Q^S(t)$. The liquid domain is $Q^L(t) = Q \setminus \overline{Q^S(t)}$.

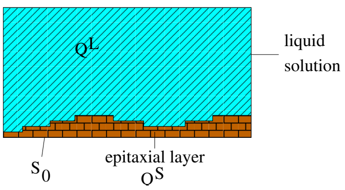


Figure 1: Liquid Phase Epitaxy

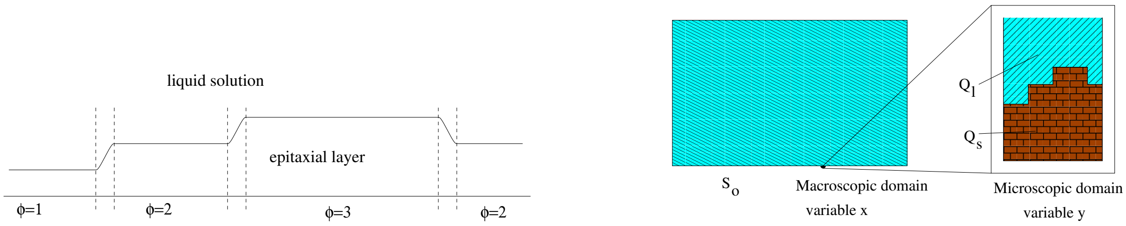
The key idea of our two scale model is, that we describe the evolution of the microstructures in terms of a microscopic space variable y, while macroscopic processes are modeled in terms of a macroscopic space variable x. First we have to define suitable domains for x and y, see Figure 2(b). We let $x \in Q$. The only purely macroscopic process is the transport of molecules in the liquid, far away from the interface. Thus, we consider Q to be fully occupied by the liquid solution and shift the free boundary problem, i.e. the evolution of the layer, to the microscopic part of the model.

At every macroscopic point $x \in S_0$, we define a microscopic domain $Y \times (0, \infty)$, see Figure 2(b), where $Y = [0, 1]^2$ is a two dimensional periodicity cell. Each microscopic domain consists of two parts: the upper, Q_l, is filled with the liquid solution and the lower, Q_s, is occupied by the solid layer. For the description of the interface between these two parts, we introduce a phase field function $\phi\colon Y \to [0, \infty)$, see Figure 2(a), which we interpret as the number of mono–molecular layers over a point on Y. If we denote the height of one mono–molecular layer by h_A, then the interface between liquid solution and solid layer is given as the graph of the function $h_A\phi$. The natural values of ϕ would be the integers, but we allow ϕ to take on real values in a neighborhood of a step which enables a smooth transition from step to step.

Using ϕ, we define the microscopic domains Q_l and Q_s and the free interface Γ for fixed $x \in S_0$ and $t \in I = [0, T]$ by

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

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



(a) The phase field.

(b) Macro- / micro-domains: One microscopic domain for every macroscopic point $x \in S_0$.

Figure 2: Description of the interface

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 [7].

The unknown quantities are:

$v(t,x,y), V(t,x)$	fluid velocity	$p(t,x,y), P(t,x)$	pressure
$\phi(t,x,y)$	phase field	$u(t,x,y)$	elastic displacement
$C^{\mathcal{V}}(t,x)$	volume concentration of molecules in the liquid solution	$c_s(t,x,y)$	surface concentration of adatoms

Capital letters denote purely macroscopic quantities, small letters indicate quantities depending on x and y (all these variables also depend on time). The velocity v is the term of order ε in the inner expansion of the homogenization procedure; the term of order 1 vanishes. All these other quantities are of lowest order in ε in their corresponding expansions. The model is composed of:

- Macroscopic Navier-Stokes equations and a convection-diffusion equation in $I \times Q$:

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

$$\partial_t C^{\mathcal{V}} + V \cdot \nabla_x C^{\mathcal{V}} - D^{\mathcal{V}} \Delta_x C^{\mathcal{V}} = 0. \tag{2}$$

  The constant $\eta > 0$ in (1) denotes the viscosity of the fluid and $D^{\mathcal{V}} > 0$ is a diffusion constant. Furthermore, we have coupling conditions to the microscopic problems on $I \times S_0$:

$$D^{\mathcal{V}} \partial_{x_3} C^{\mathcal{V}}|_{x_3=0} = \left(\frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{\bar{c}_s}{\tau_s} \right), \tag{3}$$

$$V = 0, \tag{4}$$

  Here, $\bar{c}_s(t,x) = \int_Y c_s(t,x,y)\,\mathrm{d}y$ and $\tau^{\mathcal{V}} > 0$ and $\tau_s > 0$ describe the rates of adsorption and desorption of adatomes from and to the liquid solution. The boundary condition (4) is a consequence of the asymptotic matching of inner and outer expansions of the velocity. Thus, the Navier-Stokes system (1) decouples from the other equations. Therefore, we may consider the velocity field V and the pressure P as given functions. To ensure the well–posedness we complete this part of the model by initial conditions and standard boundary conditions on $I \times (\partial Q \setminus S_0)$.

- A microscopic Stokes system at every fixed point $x \in S_0$ and time $t \in I$:

$$\left.\begin{aligned} \operatorname{div}_y v &= 0, \\ -\eta \Delta_y v + \nabla_y p &= 0, \end{aligned}\right. \quad \text{in } Q_l. \tag{5}$$

  We assume periodic boundary conditions for v with respect to y_1, y_2. Furthermore, we have two coupling conditions. On the free boundary Γ this is

$$v = v_\Gamma := -J_s^{-1} \left(\frac{1}{\varrho_V} - \frac{1}{\varrho_E} \right) \left(\frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{c_s}{\tau_s} \right) e_3, \tag{6}$$

where the factor J_s is the density of a surface measure for the interface parameterized over S_0. ϱ_V and ϱ_E are the densities of the liquid solution and the solid layer, respectively. For $y_3 \to \infty$ we match v, p and V, P asymptotically in the following way:

$$\lim_{y_3 \to \infty} \eta \left(\nabla_y v + (\nabla_y v)^\top \right) e_3 - p e_3 = \eta \left(\nabla_x V|_{x_3=0} + (\nabla_x V)^\top|_{x_3=0} \right) e_3 - P|_{x_3=0} e_3. \tag{7}$$

- A microscopic elastic equation to be solved for every $x \in S_0$, $t \in I$

$$-\operatorname{div}_y \sigma_y(u) = 0, \quad \text{in } Q_s, \tag{8}$$

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

$$u = b, \qquad \text{for} \quad y \in \tilde{\Gamma} := Y \times \{0\}, \tag{9}$$

periodic boundary conditions for u with respect to y_1, y_2, and the coupling

$$\sigma_y(u) n_{ys} + 2\eta\, e_y(v)\, n_{yl} - p n_{yl} = 0, \quad \text{on } \Gamma, \tag{10}$$

to the Stokes system. 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}.

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

$$\tau \xi^2 \partial_t \phi - \xi^2 \Delta_y \phi + f'(\phi) + q(c_s, u, \phi) = 0, \tag{11}$$

$$\partial_t c_s + \varrho_s h_A \partial_t \phi - D_s \Delta_y c_s = \frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{c_s}{\tau_s}, \tag{12}$$

with initial conditions

$$c_s(0, x, y) = c_{s,ini}(x, y), \qquad \phi(0, x, y) = \phi_{ini}(x, y), \tag{13}$$

and periodic boundary conditions with respect to y_1, y_2. Note, that these equations are defined on a surface and are thus two-dimensional in space. $D_s > 0$ denotes the diffusivity for the surface diffusion, $\varrho_s > 0$ the surface density of adatoms, $\tau > 0$ a time relaxation parameter, $\xi > 0$ describes the thickness of the smooth step transition regions. The function f is a multi-well potential with minima at integer values, e.g. $f(\phi) = -\cos(2\pi\phi)$, and

$$q(c_s, u, \phi) = \frac{\xi R \mathcal{T} \varrho_s}{c_{\text{eq}} \gamma \beta}(c_{eq} - c_s) g(\phi) + \frac{\xi h_A \varrho_s}{2 c_{\text{eq}} \gamma \beta} \sigma_y(u) : e_y(u), \tag{14}$$

with gas constant R, temperature $\mathcal{T}$, equilibrium concentration c_{eq}, step stiffness γ, and a calibration parameter β. For the function g we suppose $g(\phi) = 0$ for $\phi \in \mathbb{N}_0$, e.g. $g(\phi) = 1 - \cos(2\pi\phi)$. This ensures that the corresponding Gibbs-Thomson condition is only valid in the neighborhood of a step, see [14].

3 The Iterative Procedure

The two scale formulation is an alternative approach for solving the model equations numerically compared to direct simulation. The computation of the microstructure has to be done on representative periodicity cells which shrink, from the macroscopic point of view, to single points. The microscopic quantity c_s occurs in a coupling term in the macroscopic equations in an averaged form. As a consequence of that approach it is possible to choose a much coarser grid in the macroscopic domain compared to a direct simulation approach. It is not necessary to resolve the microstructure. The price to pay is that in every macroscopic grid point on the growing interface one microscopic problem has to be solved. An adaptive strategy as in [18], which reduces the computation effort significantly, might be applicable.

Due to to the boundary condition (4) the Navier–Stokes system decouples from the rest of the model equations. As a consequence the macroscopic velocity V and the macroscopic pressure P can be computed in advance. The subsequent iterative procedure consists in fact of two encapsulated iterations: The remaining macroscopic convection–diffusion equation and the coupled microscopic problem (composed of phase field, Stokes and Elasticity system) are solved in turns where in each step, the microscopic problem is again solved iteratively. More precisely, it reads as follows:

1. Solve the decoupled macroscopic Navier–Stokes system (1), (4) in the domain $I \times Q$. We get V and P.

2. Choose an initial phase field ϕ_0 that describes the free boundary Γ_0 and choose an initial surface concentration $c_{s,0}$.

3. Calculate the mean value $\bar{c}_{s,0}$. Solve the macroscopic convection–diffusion equation (2), (3) in $I \times Q$ to get $C_0^{\mathcal{V}}$.

4. Solve the microscopic equations by an encapsulated iteration procedure in order to get a good approximation for ϕ and c_s:

   (a) Set $\phi^0 := \phi_0$ and $c_s^0 := c_{s,0}$. Calculate v^0 and p^0 as solutions of the microscopic Stokes–system (5), (6), (7).

   (b) Solve the microscopic elasticity system (8), (9), (10) with data v^0, p^0 and ϕ^0 in order to get u^0.

   (c) Calculate the new quantities ϕ^1 and c_s^1 from the system (11), (12) with coupling data u^0 and $C_0^{\mathcal{V}}$.

   (d) Restart in 4.(a) with ϕ^1 and c_s^1 instead of ϕ^0 and c_s^0. Continue the microscopic iteration until a satisfactoring approximation ϕ^N and c_s^N is reached.

5. Restart in 3. with the data $c_{s,1} := c_s^N$ and proceed with $\phi_1 := \phi^N$ instead of ϕ_0 ...

In the following sections we prove the existence and uniqueness of solutions for every single problem on its own, considering the coupling data as given functions. These results ensure, that every step in the above iteration is meaningful. The setting of function spaces is chosen in such a way that each iterative step takes place in the same spaces. In particular this means that all functions do not loose regularity during the process.

However, it is not clear at this stage if the above procedure converges in some sense. This question is closely related to the solvability of the fully coupled model equations which still is an open problem.

4 Solvability of the Macroscopic Equations

In this section we discuss the solvability of the well known Navier–Stokes equation (1), (4) and convection–diffusion equation (2), (3) in $I \times Q$. Since the Navier–Stokes equations decouple from the rest of the model, the macroscopic velocity field V and the macroscopic pressure P can be computed in advance before studying these other equations. We refer to [24] where an overview on solvability results for different boundary conditions can be found. Here, we assume that we have solutions $V \in C^{\alpha}(I, C^1(Q))$, with some $\alpha > 0$, and $P \in C^{\alpha}(I, C^0(Q))$, see [24], Ch. 3.5.2, Remark 3.8.

The convection-diffusion equation (2) together with the coupling (3) and homogeneous Neumann conditions on $Q \setminus S_0$ has been investigated in [6]. Thus, we only formulate the results here. The **weak formulation of the problem** is given by:

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

$$\int_I \left(\langle \partial_t C^{\mathcal{V}}, u \rangle + \int_Q (V \cdot \nabla C^{\mathcal{V}} u + D^{\mathcal{V}} \nabla C^{\mathcal{V}} \cdot \nabla u) \, dx \right) dt = \int_{I \times S_0} \left(\frac{\bar{c}_s}{\tau_s} - \frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} \right) u \, ds_x \, dt, \tag{15}$$

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

Theorem 4.1.

1. *For given* $\bar{c}_s \in L_2(I \times S_0)$, $C^{\mathcal{V}}_{ini} \in L_2(Q)$, *problem (15) has a unique solution.*

2. *Suppose further, that the initial condition* $C^{\mathcal{V}}_{ini} \in H^2(Q)$. *Then for* $\bar{c}_s \in C^0(I, C^1(S_0))$ *the solution* $C^{\mathcal{V}}$ *of (15) is an element of* $C^1((0,T), L_2(Q)) \cap C^0((0,T), H^1(Q))$.

Proof. 1. This was proven in [6].

2. This follows from Theorem 11 in [19], p.417.

□

5 Solvability of the Microscopic Equations

The microscopic equations (5)-(13) are fully coupled and questions about solvability and regularity of solutions are still open. In this paper, we restrict to the single steps introduced in the iterative procedure in section 3 and investigate existence, uniqueness and regularity of solutions of the corresponding single problems. Throughout this section, all quantities and equations are considered at a fixed macroscopic point $x \in S_0$, even if not explicitly stated everywhere, with given $C^{\mathcal{V}}$. The macroscopic quantity $C^{\mathcal{V}}(\cdot, x)$ at a fixed point $x \in S_0$ is constant with respect to y.

Note first of all, that the problem (11), (12), (13) for ϕ and c_s is an evolution problem, while the Stokes problem (5), (6), (7) and the elastic problem (8), (9), (10) are quasi-stationary: v, p and u depend on time, but the corresponding equations do not include any time derivatives. Nevertheless, the regularity in time for *all* of these solutions (after proven to be existent) has to be investigated. Since the domains $Q_l = Q_l(t)$ and $Q_s = Q_s(t)$ depend also on time, it is therefore necessary to introduce time-independent domains $\hat{Q}_l$ and $\hat{Q}_s$, together with corresponding (time dependent) domain transformations

$$\Psi_l(t) \colon \hat{Q}_l \to Q_l(t), \qquad \Psi_s(t) \colon \hat{Q}_s \to Q_s(t),$$

which will be defined properly in the sections 5.1 and 5.2. For functions v, p and u, defined on $Q_l(t)$ and $Q_s(t)$ respectively, $\hat{v} := v \circ \Psi_l$, $\hat{p} := p \circ \Psi_l$ and $\hat{u} := u \circ \Psi_s$ denote their counterparts, defined on the time-independent domains $\hat{Q}_l$ and $\hat{Q}_s$.

Concerning the solvability of the single microscopic problems, we prove the existence of the following microscopic solution operators at a fixed point $x \in S_0$ and for given $C^{\mathcal{V}}(\cdot, x) \in C^\alpha(I)$, for $0 < \alpha < \frac{1}{4}$:

- For the Stokes problem:

$$\mathcal{S}_1 : \left[C^\alpha(I, C^2(Y))\right]^2 \to C^\alpha(I, C^2(Y) \times [W^2_r(\hat{Q}_{lK})]^3 \times W^1_r(\hat{Q}_{lK})) : (\phi, c_s) \mapsto (\phi, \hat{v}, \hat{p}),$$

  where

$$Q_{lK} := \{y \in Q_l |\, y_3 < h_A \phi(y_1, y_2) + K\}, \quad K > 0, \qquad \text{and} \qquad \hat{Q}_{lK} := \Psi_l^{-1}(Q_{lK}).$$

  The phase field ϕ is unchanged by the application of $\mathcal{S}_1$, which is necessary in order to define the composition $\mathcal{S}_2 \circ \mathcal{S}_1$.

- For the elastic problem:

$$\mathcal{S}_2 : C^\alpha(I, C^2(Y) \times [W^2_r(\hat{Q}_{lK})]^3 \times W^1_r(\hat{Q}_{lK})) \to C^\alpha(I, [W^2_r(\hat{Q}_s)]^3) : (\phi, \hat{v}, \hat{p}) \mapsto \hat{u}.$$

- For the phase field equations:

$$\mathcal{S}_3 : C^\alpha(I, [W^2_r(\hat{Q}_s)]^3) \to \left[C^{1+\alpha, 2+2\alpha}(I \times Y)\right]^2 : \hat{u} \mapsto (\phi, c_s),$$

  where

$$C^{1+\alpha,2+2\alpha}(I \times Y) = \{w \in C^{1,2}(I \times Y) : \partial_t w, \partial_{y_i y_j} w \in C^{\alpha, 2\alpha}(I \times Y),\ i,j = 1,2\},$$
$$C^{\beta,2\beta}(I \times Y) = C^\beta(I, C^0(Y)) \cap C^0(I, C^{2\beta}(Y)), \quad 0 \le \beta \le 1.$$

The functions $(v,p) = \mathcal{S}_1(\phi, c_s) \circ \Psi_l^{-1}$ and $u = \mathcal{S}_2(\phi, v, p) \circ \Psi_s^{-1}$ have to be understood as solutions in the distributional sense of their corresponding problems, while $(\phi, c_s) = \mathcal{S}_3(\hat{u})$ are indeed classical solutions. The C^2-regularity of ϕ with respect to the space variable y cannot be weakened in this setting because ϕ describes parts of the boundaries of the domains of the Stokes and the elastic equations: With a boundary of regularity less than C^2 we cannot prove the existence of solutions in spaces of the form W_r^2 and W_r^1 for v, u and p, respectively.

We remark, that the solution operator for the fully coupled problem is described by the composition of the operators $\mathcal{S}_3 \circ \mathcal{S}_2 \circ \mathcal{S}_1$ which maps $\left[C^\alpha(I, C^2(Y))\right]^2$ into itself if we choose $r > \frac{5}{1-2\alpha}$.

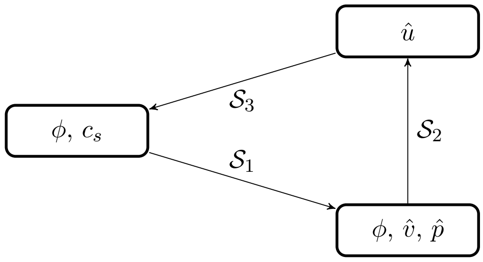


Figure 3: The microscopic iteration, with given $C^{\mathcal{V}}$.

Concerning the notation: In some of the following estimates, the constant depends on the boundary of the corresponding domain and thus on ϕ. In these cases, we will state this explicitly. In all estimates, where nothing like that is mentioned, the constants are independent of ϕ and of the other unknowns.

5.1 The Microscopic Stokes System and the Operator $\mathcal{S}_1$

We consider (5), (6) and (7). For simplicity, we will *firstly* look for solutions of the problem on the semi–infinite domain Q_l in suitable Hilbert spaces and *secondly* discuss the regularity of this solution on the bounded subdomain $Q_{lK} \subset Q_l$. This is done since we are not interested in the behavior of v and p at infinity but only on their regularity on Γ, due to the coupling to the elastic equation.

We prove the existence of a solution that satisfies

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

which means that the pressure passes over continuously from the macroscopic to the microscopic part of the model. Thus (7) is modified to

$$\lim_{y_3 \to \infty} \left(\nabla_y v + (\nabla_y v)^\top\right) e_3 = \left(\nabla_x V|_{x_3=0} + (\nabla_x V)^\top|_{x_3=0}\right) e_3 = \left(\partial_{x_3} V_1, \partial_{x_3} V_2, 0\right)^\top\Big|_{x_3=0} =: \mathbf{a},$$

using the boundary condition (4), which leads to $\partial_{x_1} V|_{x_3=0} = \partial_{x_2} V|_{x_3=0} = 0$ and implies together with $\operatorname{div} V = 0$ that $\partial_{x_3} V_3|_{x_3=0} = 0$. For some sufficiently large constant $M > h_A \|\phi\|_{L_\infty(Y)}$, we define

$$\tilde{v}(y) := \begin{cases} \mathbf{a}\,(y_3 - M), & y_3 \geq M \\ 0, & y_3 < M \end{cases}.$$

Obviously, we have almost everywhere in Q_l: $\lim_{y_3\to\infty} \left(\nabla_y \tilde{v} + (\nabla_y \tilde{v})^\top\right) e_3 = \mathbf{a}, \quad \operatorname{div} \tilde{v} = 0, \quad \Delta \tilde{v} = 0.$

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

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

where v_Γ is given by (6). We introduce an artificial boundary $\hat{\Gamma} := \{y \in Q_l | y_3 = h_A \phi(y_1, y_2) + K\}$, with some positive constant K. The surface $\hat{\Gamma}$ is the upper boundary of the bounded domain Q_{lK}. The following Lemma guaranties that we can transform the inhomogeneous Dirichlet condition (6) on Γ into a homogeneous one:

Lemma 5.1. *Suppose that $Y = [0,1]^2$. Then, there exists a Y–periodic function $u \in [H^1(Q_{lK})]^3$ such that $u|_\Gamma = v_\Gamma - \bar{v}$, $u|_{\hat{\Gamma}} = 0$ and $\operatorname{div} u = 0$. Furthermore,*

$$\|u\|_{H^1(Q_{lK})} \leq c\left(1 + \|\phi\|_{C^2(Y)}\right)^3 \|v_\Gamma - \bar{v}\|_{H^{1/2}(Y)}.$$

Proof. In a *first step*, we consider the time independent domain $\hat{Q}_{lK} := Y \times [0, K]$ and the transformation

$$\Psi_l(t)\colon \hat{Q}_{lK} \to Q_{lK}(t)\colon \hat{y} = (\hat{y}_1, \hat{y}_2, \hat{y}_3)^\top \mapsto y := (\hat{y}_1, \hat{y}_2, \hat{y}_3 + h_A\phi(t, \hat{y}_1, \hat{y}_2))^\top . \tag{16}$$

We transform a vector field on Q_{lK} into a vector field on $\hat{Q}_{lK}$ by using the Piola transform for vectors, which is defined for fixed $\hat{y} \in \hat{Q}_{lK}$, $y = \Psi_l(\hat{y}) \in Q_{lK}$ by

$$\mathcal{P}\colon \mathbb{R}^3 \to \mathbb{R}^3\colon v(y) \mapsto v^{\mathcal{P}}(\hat{y}) := \mathrm{Cof}(D\Psi_l(\hat{y}))^\top v(y),$$

where $\mathrm{Cof}(D\Psi_l(\hat{y}))^\top$ is the transposed of the Cofactor matrix of $D\Psi_l$. We recall that

$$\mathrm{div}_{\hat{y}}\, v^{\mathcal{P}} = \det(D\Psi_l)\, \mathrm{div}_y\, v = \mathrm{div}_y\, v, \qquad \int_{\partial\hat{Q}_{lK}} v^{\mathcal{P}} \cdot n \,\mathrm{d}\hat{s} = \int_{\partial Q_{lK}} v \cdot n \,\mathrm{d}s,$$

see e.g. [22], Ch.1.4. We intend to prove that there exists a Y–periodic function $w^{\mathcal{P}} \in [H^1(\hat{Q}_{lK})]^3$ such that $w^{\mathcal{P}}|_{y_3=0} = (v_\Gamma - \bar{v})^{\mathcal{P}}$ and $w^{\mathcal{P}}|_{y_3=K} = 0$. Therefore, we consider the following boundary value problem

$$\Delta w^{\mathcal{P}} = 0, \quad \text{in } \hat{Q}_{lK}, \qquad w^{\mathcal{P}} = \begin{cases} 0 & \text{for } \hat{y}_3 = K, \\ (v_\Gamma - \bar{v})^{\mathcal{P}} & \text{for } \hat{y}_3 = 0, \\ Y-\text{periodic} & \text{with respect to } (\hat{y}_1, \hat{y}_2) \in \partial Y. \end{cases} \tag{17}$$

Using the representation as a Fourier series in terms of $(\hat{y}_1, \hat{y}_2) \in Y$

$$w^{\mathcal{P}}(\hat{y}) = \sum_{k,l \in \mathbb{Z}} b_{kl}(\hat{y}_3)\, e^{2\pi i(k\hat{y}_1 + l\hat{y}_2)},$$

a solution of (17) can be calculated explicitly. This solution satisfies

$$\|w^{\mathcal{P}}\|_{H^1(\hat{Q}_{lK})} \le c\|(v_\Gamma - \bar{v})^{\mathcal{P}}\|_{H^{1/2}(Y)} \le c\left(1 + \|\phi\|_{C^2(Y)}\right)\|v_\Gamma - \bar{v}\|_{H^{1/2}(Y)}. \tag{18}$$

In the *second step*, we prove the existence of a divergence free Y–periodic function in $H^1(\hat{Q}_{lK})$ with the boundary values (17). From the construction of $\bar{v}$, the periodicity of $w^{\mathcal{P}}$ and the properties of the Piola transform it follows

$$\int_{\hat{Q}_{lK}} \mathrm{div}\, w^{\mathcal{P}} \,\mathrm{d}\hat{y} = \int_{\partial\hat{Q}_{lK}} w^{\mathcal{P}} \cdot n \,\mathrm{d}\hat{s} = 0.$$

We follow the ideas of [12], Ch.I, §2.2 and get a function $v^{\mathcal{P}} \in [H^1_0(\hat{Q}_{lK})]^3$ with

$$\mathrm{div}\, v^{\mathcal{P}} = \mathrm{div}\, w^{\mathcal{P}}, \qquad \|\nabla v^{\mathcal{P}}\|_{L_2(\hat{Q}_{lK})} \le c\|\,\mathrm{div}\, w^{\mathcal{P}}\|_{L_2(\hat{Q}_{lK})}. \tag{19}$$

Since all functions in $[H^1_0(\hat{Q}_{lK})]^3$ are Y–periodic, this is also true for $v^{\mathcal{P}}$ and thus also for $u^{\mathcal{P}} := w^{\mathcal{P}} - v^{\mathcal{P}}$. (18), (19) and the Poincaré–Friedrichs inequality for $v^{\mathcal{P}}$ imply

$$\|u^{\mathcal{P}}\|_{H^1(\hat{Q}_{lK})} \le c\,\left(1 + \|\phi\|_{C^2(Y)}\right)\,\|v_\Gamma - \bar{v}\|_{H^{1/2}(Y)}. \tag{20}$$

The constant occurring in the Poincaré–Friedrichs inequality only depends on the diameter of $\hat{Q}_{lK}$. Thus the constant c in (20) is independent of $u^{\mathcal{P}}$, v_Γ and ϕ.

In the *third and last step*, we use the inverse Piola transform to define

$$u(y) = \mathcal{P}^{-1}\, u^{\mathcal{P}}(\hat{y}).$$

This is the required function which satisfies the boundary conditions and is divergence free by construction. By using the product and the chain rule we get u Y–periodic in $[H^1(Q_{lK})]^3$ with

$$\|u\|_{H^1(Q_{lK})} \le c\left(1 + \|\phi\|_{C^2(Y)}\right)^2\|u^{\mathcal{P}}\|_{H^1(\hat{Q}_{lK})} \le c\left(1 + \|\phi\|_{C^2(Y)}\right)^3\|v_\Gamma - \bar{v}\|_{H^{1/2}(Y)}.$$

□

We extend u to Q_l by setting $u(y) = 0$ for $y \in Q_l \setminus Q_{lK}$. Obviously, $u \in [H^1(Q_l)]^3$ with $\operatorname{div} u = 0$. We return to the Stokes problem (5), (6), (7). For the function $z := v - \bar{v} - \tilde{v} - u$ we consider the problem

$$\left.\begin{aligned} -\eta\Delta z + \nabla p &= \eta\Delta u, \\ \operatorname{div} z &= 0, \end{aligned}\right\} \quad \text{in } Q_l, \tag{21}$$

$$z = 0 \quad \text{on } \Gamma, \quad \lim_{y_3\to\infty} e(z)e_3 = 0, \quad z \text{ is } Y-\text{periodic}, \tag{22}$$

where $e(z) = \frac{1}{2}(\nabla z + (\nabla z)^\top)$. If z solves (21), then v is a solution of the original problem (5). Let

$$\mathcal{X} := \left\{ w|_{Q_l} \,\middle|\, w(\cdot,\cdot,y_3) \text{ is } Y-\text{periodic in } C^\infty(\mathbb{R}^2),\ w(y_1,y_2,\cdot) \in C_0^\infty(\mathbb{R}),\ w|_\Gamma = 0,\ \operatorname{div} w = 0 \right\}.$$

We take the $\mathbb{R}^3$-scalar-product of $w \in \mathcal{X}$ with the first equation of (21), integrate over Q_l and integrate by parts to find

$$\int_{Q_l} 2\eta\, e(z) : e(w)\, \mathrm{d}y = -\int_{Q_l} 2\eta\, e(u) : e(w)\, \mathrm{d}y.$$

Note, that the pressure term vanishes due to $\operatorname{div} w = 0$ for $w \in \mathcal{X}$, and that the property $\operatorname{div} z = 0$ implies the identity $\Delta z = \operatorname{div}(e(z))$. Let X be the closure of $\mathcal{X}$ with respect to the norm

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

which indeed is a norm on $\mathcal{X}$ due the condition $w|_\Gamma = 0$. Note, that X might not be equal to the closure of $\mathcal{X}$ with respect to the H^1–norm, since the domain Q_l is unbounded. X is a Hilbert space. A **weak formulation of the problem** (21), (22) is given by
Find $z \in X$ such that

$$a(z,w) = \ell(w), \quad \text{for all } w \in X, \tag{23}$$

where $a(z,w) := \int_{Q_l} 2\eta\, e(z) : e(w)\, \mathrm{d}y$, $\quad \ell(w) := -\int_{Q_l} 2\eta\, e(u) : e(w)\, \mathrm{d}y$.

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

Theorem 5.2. *For any fixed time $t \in [0,T]$ and any point $x \in S_0$, (23) has a unique solution $z \in X$. Furthermore, there exists a function $p \in L_{2,\mathrm{loc}}(Q_l)$ with $\lim_{y_3\to\infty} p = P|_{x_3=0}$ such that*

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

in the distributional sense in Q_l. Concerning the semi–infinite domain Q_l, z satisfies the estimate

$$\|z(t,x)\|_X \le c_1 \left(1 + \|\phi(t,x)\|_{C^2(Y)}\right)^3 \left(|C^{\mathcal{V}}(t,x)| + \|c_s(t,x)\|_{H^{1/2}(Y)}\right). \tag{24}$$

Restricting all functions to the bounded subdomain $Q_{lK} \subset Q_l$, we have

$$\begin{aligned} &\|v(x,t)\|_{H^1(Q_{lK})} + \|p(x,t)\|_{L_2(Q_{lK})} \\ &\quad \le c_2 \left(1 + \|\phi(x,t)\|_{C^2(Y)}\right)^4 \left(|C^{\mathcal{V}}(t,x)| + \|c_s(t,x)\|_{H^{1/2}(Y)}\right) + c_3 \left|\nabla V(t,x)\right| + C(P(t,x)). \end{aligned} \tag{25}$$

Before we prove this theorem we state a version of the First Korn inequality:

Lemma 5.3. *Let $\Omega = Y \times \mathbb{R}$ with $Y = [0,1]^2$ and let*

$$\mathcal{W} = \left\{ w|_\Omega \mid w(\cdot,\cdot,y_3) \text{ is } Y-\text{periodic in } C^\infty(\mathbb{R}^2),\ w(y_1,y_2,\cdot) \in C_0^\infty(\mathbb{R}),\ w(y_1,y_2,0) = 0 \right\}.$$

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:

$$\|\nabla u\|_{L_2(\Omega)}^2 \le 2\|e(u)\|_{L_2(\Omega)}^2.$$

The proof can be found in [8]. Now we prove Theorem 5.2:

Proof. The bilinear form a is continuous. It is also X-elliptic: Extend z to the strip $Y \times \mathbb{R}$ by setting

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

The extended function z belongs to the space W defined in Lemma 5.3 and we get

$$\|\nabla z\|^2_{L_2(Q_l)} \leq 2\|e(z)\|^2_{L_2(Q_l)}.$$

Hence a is X-elliptic and due to the Lax-Milgram Theorem, there is a unique solution z of (23) which satisfies

$$\|z\|_X \leq c\|\ell\|_{X'}.$$

Existence of p:

For the solution z of (23) the mapping $a(z, \cdot) - \ell(\cdot)$ belongs to the space $[H^{-1}(Q_l)]^3$ with

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

Since $\{\nu \in [C_0^\infty(Q_l)]^3 \mid \operatorname{div} \nu = 0\} \subset \mathcal{X}$ holds, Propositions 1.1 and 1.2 in [24], Ch.1, §1, pp. 14-15, imply that there exists a $p \in L_{2,\mathrm{loc}}(Q_l)$, uniquely defined up to a constant, such that

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

in the distributional sense in Q_l. It remains to prove that we can choose this constant in such a way that

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

Therefore it suffices to show that p becomes constant if y_3 tends to infinity. For $N \in \mathbb{N}$ and $w \in [H_0^1(Q_l)]^3$ we define

$$\Omega_N := \{y \in Q_l \mid y_3 > N\}, \quad w_N(y_1, y_2, y_3) := w(y_1, y_2, y_3 - N).$$

Clearly $w_N \in [H_0^1(\Omega_N)]^3$. If N is sufficiently large we have

$$-\eta \Delta z + \nabla p = 0 \quad \text{in } H^{-1}(\Omega_N),$$

and thus

$$|\langle \nabla p, w_N \rangle_{\Omega_N}| \leq \left| \int_{\Omega_N} \nabla z : \nabla w_N \, \mathrm{d}y \right| \leq \|\nabla z\|_{L_2(\Omega_N)} \|\nabla w_N\|_{L_2(\Omega_N)}.$$

The last expression tends to zero for $N \to \infty$ since $\|\nabla z\|_{L_2(Q_l)} < \infty$. It follows that $\nabla p \to 0$ in $H^{-1}(\Omega_N)$ which implies, together with VI. Satz in [27], p.88, that p becomes constant if y_3 tends to infinity.

Estimate for the right hand side:

We proved in Lemma 5.1 that

$$c\|\ell\|_{V'} \leq c\|\nabla u\|_{L_2(Q_l)} \leq c \left(1 + \|\phi\|_{C^2(Y)}\right)^3 \|v_\Gamma - \hat{v}\|_{H^{1/2}(Y)}.$$

Furthermore it follows from the definition of v_Γ, see (6), that

$$\|\hat{v}\|_{H^{1/2}(Y)} = \frac{\int_\Gamma v_\Gamma \cdot n \, \mathrm{d}s}{\int_\Gamma n_3 \, \mathrm{d}s} \|1\|_{L_2(Y)} \leq c \left(|C^{\mathcal{V}}| + \|c_s\|_{L_2(Y)}\right)$$

and

$$\|v_\Gamma\|_{H^{1/2}(Y)} \leq c \left(|C^{\mathcal{V}}| + \|c_s\|_{H^{1/2}(Y)}\right).$$

Restriction to Q_{lK}:

For the velocity it follows from (24), the Poincaré-Friedrichs inequality for z in Q_{lK}, and the definition of $\tilde{v}$ and $\bar{v}$

$$
\begin{aligned}
\|v\|_{H^1(Q_{lK})} &\le \|z+u+\bar{v}+\tilde{v}\|_{H^1(Q_{lK})} \\
&\le c_1\left(1+\|\phi\|_{C^2(Y)}\right)^3\left(|C^{\mathcal{V}}|+\|c_s\|_{H^{1/2}(Y)}\right)+c_2|a| \\
&\le c_1\left(1+\|\phi\|_{C^2(Y)}\right)^3\left(|C^{\mathcal{V}}|+\|c_s\|_{H^{1/2}(Y)}\right)+c_2\Big|\nabla V\Big|_{x_3=0}.
\end{aligned}
$$

It follows from Proposition 1.2 in [24], Ch. I, §1, pp.14-15, that $p \in L_2(Q_{lK})$. The pressure can be estimated in the following way: We consider the transformation Ψ_l, see (16), and define $\hat{p} = p \circ \Psi_l \in L_2(\hat{Q}_{lK})$. We have $\nabla \hat{p} \in [H^{-1}(\hat{Q}_{lK})]^3$ with

$$
\|\nabla \hat{p}\|_{H^{-1}(\hat{Q}_{lK})} \le c\left(1+\|D\phi\|_{L_\infty(Y)}\right)\|\nabla p\|_{H^{-1}(Q_{lK})}.
$$

It follows again from Proposition 1.2 in [24], Ch. I, §1, pp.14-15:

$$
\|p\|_{L_2(Q_{lK})/\mathbb{R}} = \|\hat{p}\|_{L_2(\hat{Q}_{lK})/\mathbb{R}} \le c\|\nabla \hat{p}\|_{H^{-1}(\hat{Q}_{lK})} \le c\left(1+\|D\phi\|_{L_\infty(Y)}\right)\|\nabla p\|_{H^{-1}(Q_{lK})}.
$$

The constant c depends on $\hat{Q}_{lK}$ but not on ϕ. We split p now additively in the following way:

$$
p = p_0 + p_1,
$$

with $\int_{Q_{lK}} p_0 \, \mathrm{d}y = 0$ and a constant $p_1 = p - p_0$ which depends on $P|_{x_3=0}$. For p_0 there holds

$$
\|p_0\|_{L_2(Q_{lK})} = \|p\|_{L_2(Q_{lK})/\mathbb{R}}.
$$

This implies

$$
\begin{aligned}
\|p\|_{L_2(Q_{lK})} &\le c\left(1+\|D\phi\|_{L_\infty(Y)}\right)\|\nabla p\|_{H^{-1}(Q_{lK})} + C(P|_{x_3=0}) \\
&\le c_1\left(1+\|\phi\|_{C^2(Y)}\right)^4\left(|C^{\mathcal{V}}|+\|c_s\|_{H^{1/2}(Y)}\right)+c_2\Big|\nabla V\Big|_{x_3=0} + C(P|_{x_3=0}).
\end{aligned}
$$

□

We study now the regularity of the restrictions of v and p to Q_{lK} applying classical regularity results for the Stokes problem, namely Propositions 2.2 and 2.3 in [24], Ch.I, §2, pp.33-35. These results concern the Stokes equations with Dirichlet boundary conditions and can be used to prove the following theorem:

Theorem 5.4. *Suppose $2 \le r < \infty$, $\phi \in C^2(\bar{Y})$ with $\|\phi\|_{C^2(Y)} \le \kappa$, for some constant $\kappa > 0$, and $c_s \in W_r^{2-1/r}(Y)$. Then, for fixed $x \in S_0$, $t \in I$, the solution $(v,p)(t) = \mathcal{S}_1(\phi, c_s)(t)$ of the Stokes problem satisfies $v \in \left[W_r^2(Q_{lK})\right]^3$, $p \in W_r^1(Q_{lK})$, together with the a priori estimate*

$$
\begin{aligned}
&\|v(x,t)\|_{W_r^2(Q_{lK})} + \|p(x,t)\|_{W_r^1(Q_{lK})} \\
&\qquad \le c(\kappa)\Big(\|c_s(t,x)\|_{W_r^{2-1/r}(Y)} + |C^{\mathcal{V}}(t,x)| + \big|\nabla V(t,x)\big| + C(P(t,x))\Big).
\end{aligned}
\tag{26}
$$

Proof. We consider a partition of unity, i.e. functions $\chi_i \in C_0^\infty(\mathbb{R}^3)$, $i = 1, \ldots, M$, with

$$
\bar{Q}_{lK} \subset \bigcup_{i=1}^M \operatorname{supp}(\chi_i), \qquad \operatorname{supp}(\chi_i) \cap Q_{lK} \neq \emptyset, \qquad \sum_{i=1}^M \chi_i(y) = 1, \quad \forall y \in \bar{Q}_{lK}.
$$

For $\operatorname{supp}(\chi_i) \cap \Gamma \neq \emptyset$ we define $\Omega_i := \{y \in \operatorname{supp}(\chi_i) : y_3 > h_A \phi(y_1,y_2)\}$ (where ϕ is extended periodically to $\mathbb{R}^2$), and $\Omega_i := \operatorname{supp}(\chi_i)$ else. Note, that v and p can be interpreted as functions in Ω_i after an eventual periodic extension to $(y_1,y_2) \in \mathbb{R}^2$ or considering the solutions of Theorem 5.2 for $y_3 > h_A\phi(y_1,y_2) + K$. The functions $\chi_i v$ and $\chi_i p$ solve the local problem

$$
\begin{aligned}
-\eta\Delta(\chi_i v) + \nabla(\chi_i p) &= -\eta\left(v\Delta\chi_i + 2\nabla v \nabla \chi_i\right) + p\nabla\chi_i, \quad \text{in } \Omega_i, \\
\operatorname{div}(\chi_i v) &= v \cdot \nabla \chi_i, \qquad \text{in } \Omega_i, \\
\chi_i v &= g_i, \qquad \text{on } \partial\Omega_i,
\end{aligned}
$$

$$\text{where} \quad g_i = \begin{cases} \chi_i v_\Gamma, & \text{for } y \in \Gamma, \\ 0, & \text{else.} \end{cases}$$

Due to $v \in [H^1(\Omega_i)]^3, p \in L_2(\Omega_i)$, a first application of Proposition 2.3 in [24], Ch.I, §2, p.35, implies that $\chi_i v \in [W_r^1(\Omega_i)]^3, \chi_i p \in L_r(\Omega_i)$ for $2 \le r \le 6$. Using this and applying the same result again gives us $\chi_i v \in [W_r^1(\Omega_i)]^3, \chi_i p \in L_r(\Omega_i)$ for any $r \ge 2$. Employ the argument a third time to get $\chi_i v \in [W_r^2(\Omega_i)]^3, \chi_i p \in W_r^1(\Omega_i)$ for any $r \ge 2$, presuming $c_s \in W_r^{2-1/r}(Y)$. Proposition 2.3 in [24], Ch.I, §2, p.35, also gives us an a priori estimate

$$\begin{aligned} &\|\chi_i v(x,t)\|_{W_r^2(\Omega_i)} + \|\chi_i p(x,t)\|_{W_r^1(\Omega_i)/\mathbb{R}} \\ &\qquad \le c(\kappa) \left(\|c_s(t,x)\|_{W_r^{2-1/r}(Y)} + |C^{\mathcal{V}}(t,x)| \right), \end{aligned}$$

where the constant c depends on the corresponding domain. In particular, for some $i \in \{1, \dots, M\}$, this constant depends on ϕ. In order to investigate this dependency, one has to go back to the L_r-estimates for elliptic problems by Agmon, Douglis and Nirenberg, see [2] and [3]. We use the transformation Ψ_l of Lemma 5.1 and consider the corresponding transformed local problems on $\Psi_l^{-1}(\Omega_i)$. The transformed systems of equations now have variable (and ϕ–dependent) coefficients but still are uniformly elliptic in the sense of [3]. So, Theorem 10.5 of [3] can be applied. The constant in the estimate of Theorem 10.5 in [3] depends on a bound for the corresponding norms of the coefficients and the constant of uniform ellipticity, which in our case can be estimated in terms of κ, and is else independent of ϕ. Then, Theorem 10.5 of [3] proves the above inequality. Due to $v = \sum_{i=1}^M \chi_i v, \quad p = \sum_{i=1}^M \chi_i p, \quad$ a.e. in Q_{lK}, we have

$$\|v(x,t)\|_{W_r^2(Q_{lK})} + \|p(x,t)\|_{W_r^1(Q_{lK})} \le \sum_{i=1}^M \left(\|\chi_i v(x,t)\|_{W_r^2(\Omega_i)} + \|\chi_i p(x,t)\|_{W_r^1(\Omega_i)} \right),$$

which proves (26). □

In what follows, we study the continuous dependency of v and p on the time $t \in I$. First we prove that v and p depend continuously on the coupling data. Since the coupling data is assumed to be continuous in time, this property is transferred to v and p.

Let $C^{\mathcal{V}(1)}, C^{\mathcal{V}(2)}$, $V^{(1)}, V^{(2)}$ and $P^{(1)}, P^{(2)}$ be two macroscopic volume concentrations, velocities and pressures, $(\phi^{(1)}, c_s^{(1)})$, $(\phi^{(2)}, c_s^{(2)}) \in C^2(Y) \times W_r^{1-1/r}(Y)$ and $(v^{(1)}, p^{(1)})$, $(v^{(2)}, p^{(2)})$ the corresponding solutions. Note that, if $\phi^{(1)} \ne \phi^{(2)}$, the domains of these two problems do not coincide. We transform both problems to the time independent domain $\hat{Q}_l := Y \times (0, \infty)$ or $\hat{Q}_{lK} = Y \times (0, K)$, with the help of the transformations

$$\Psi_l^{(j)}(t) : \hat{Q}_l \to Q_l^{(j)}(t), \quad \text{or} \quad \Psi_l^{(j)}(t) : \hat{Q}_{lK} \to Q_{lK}^{(j)}(t), \quad j = 1, 2,$$

defined in (16). Let be $\hat{v}^{(j)} = v^{(j)} \circ \Psi_l^{(j)}$, $\hat{p}^{(j)} = p^{(j)} \circ \Psi_l^{(j)}$, $j = 1, 2$. Then, $\hat{v}^{(j)}, \hat{p}^{(j)}$ solve

$$A(\phi^{(j)}, \hat{v}^{(j)}, \hat{p}^{(j)}) = 0, \quad \text{in } \hat{Q}_l,$$

where the differential operator $A = (A_1, A_2, A_3, A_4)$ is given for $i = 1, \dots, 3$ by

$$\begin{aligned} A_i(\phi^{(j)}, \hat{v}^{(j)}, \hat{p}^{(j)}) = &-\eta \Big(\Delta \hat{v}_i^{(j)} - h_A \partial_1 \phi^{(j)} \partial_1 \partial_3 \hat{v}_i^{(j)} - h_A \partial_2 \phi^{(j)} \partial_2 \partial_3 \hat{v}_i^{(j)} - h_A \partial_1^2 \phi^{(j)} \partial_3 \hat{v}_i^{(j)} - h_A \partial_2^2 \phi^{(j)} \partial_3 \hat{v}_i^{(j)} \Big) \\ &+ \partial_i \hat{p}^{(j)} - h_A (\delta_{1i} + \delta_{2i}) \partial_3 \hat{p}^{(j)} \partial_i \phi^{(j)}, \end{aligned}$$

with the Kronecker–delta δ_{lk}, and

$$A_4(\phi^{(j)}, \hat{v}^{(j)}, \hat{p}^{(j)}) = \operatorname{div} \hat{v}^{(j)} - h_A \partial_1 \phi^{(j)} \partial_3 \hat{v}_1^{(j)} - h_A \partial_2 \phi^{(j)} \partial_3 \hat{v}_2^{(j)},$$

together with the boundary condition

$$\hat{v}^{(j)} = -J_s^{-1} \left(\frac{1}{\varrho_V} - \frac{1}{\varrho_E} \right) \left(\frac{C^{\mathcal{V}(j)}}{\tau^{\mathcal{V}}} - \frac{c_s^{(j)}}{\tau_s} \right) e_3, \quad \text{for } y_3 = 0.$$

Lemma 5.5. *It is $\hat{v} \in C^\alpha(I, [W_r^2(\hat{Q}_{lK})]^3)$, $\hat{p} \in C^\alpha(I, W_r^1(\hat{Q}_{lK}))$ and the estimate*

$$\begin{aligned}&\|\hat{v}\|_{C^\alpha(I,W_r^2(\hat{Q}_{lK}))} + \|\hat{p}\|_{C^\alpha(I,W_r^1(\hat{Q}_{lK}))} \\ &\qquad \le c(\kappa)\Big(\|c_s\|_{C^\alpha(I,W_r^{1-1/r}(Y))} + \|\phi\|_{C^\alpha(I,C^2(Y))} + \|C^{\mathcal{V}}\|_{C^\alpha(I)} + \|\nabla_x V\|_{C^\alpha(I)} + \|P\|_{C^\alpha(I)}\Big)\end{aligned}$$

holds, where κ is an upper bound for $\|\phi(t)\|_{C^2(Y)}$ uniformly with respect to $t \in I$.

Proof. The functions $\hat{v}^{(1)} - \hat{v}^{(2)}$ and $\hat{p}^{(1)} - \hat{p}^{(2)}$ solve

$$A(\phi^{(1)}, \hat{v}^{(1)} - \hat{v}^{(2)}, \hat{p}^{(1)} - \hat{p}^{(2)}) = A(\phi^{(2)} - \phi^{(1)}, \hat{v}^{(2)}, \hat{p}^{(2)}), \quad \text{in } \hat{Q}_l,$$

with

$$\hat{v}^{(1)} - \hat{v}^{(2)} = -J_s^{-1}\left(\frac{1}{\varrho_V} - \frac{1}{\varrho_E}\right)\left(\frac{C^{\mathcal{V}(1)} - C^{\mathcal{V}(2)}}{\tau^{\mathcal{V}}} - \frac{c_s^{(1)} - c_s^{(2)}}{\tau_s}\right)e_3, \quad \text{for } \hat{y}_3 = 0,$$

and

$$\lim_{\hat{y}_3\to\infty}\Big(\nabla_{\hat{y}}(\hat{v}^{(1)} - \hat{v}^{(2)}) + \big(\nabla_{\hat{y}}(\hat{v}^{(1)} - \hat{v}^{(2)})\big)^\top\Big)e_3 = \Big(\nabla_x(V^{(1)} - V^{(2)}) + \big(\nabla_x(V^{(1)} - V^{(2)})\big)^\top\Big)\Big|_{x_3=0}e_3, \tag{27}$$

$$\lim_{\hat{y}_3\to\infty}\big(\hat{p}^{(1)} - \hat{p}^{(2)}\big) = \big(P^{(1)} - P^{(2)}\big)\Big|_{x_3=0}, \tag{28}$$

Analogously to the proof of Theorem 5.4, we find

$$\begin{aligned}&\|\hat{v}^{(1)} - \hat{v}^{(2)}\|_{W_r^2(Q_{lK})} + \|\hat{p}^{(1)} - \hat{p}^{(2)}\|_{W_r^1(Q_{lK})/\mathbb{R}} \\ &\quad \le c(\kappa)\Big(\|c_s^{(1)} - c_s^{(2)}\|_{W_r^{2-1/r}(Y)} + \|\phi^{(1)} - \phi^{(2)}\|_{C^2(Y)} + |C^{\mathcal{V}(1)} - C^{\mathcal{V}(2)}| + |\nabla_x V^{(1)} - \nabla_x V^{(2)}|\Big)\end{aligned}$$

Let further be $p^{(j)} = p_0^{(j)} + p_1^{(j)}$ with

$$\int_{Q_{lK}} p_0^{(j)}\mathrm{d}y = 0, \quad p_1^{(j)} = \int_{Q_{lK}} p^{(j)}\mathrm{d}y = \text{constant}.$$

As in the proof of Theorem 5.2, we get

$$\|\nabla(\hat{p}^{(1)} - \hat{p}^{(2)})\|_{X'} \le c(\kappa)\left(\|c_s^{(1)} - c_s^{(2)}\|_{W_r^{2-1/r}(Y)} + |C^{\mathcal{V}(1)} - C^{\mathcal{V}(2)}| + |\nabla_x V^{(1)} - \nabla_x V^{(2)}|\right),$$

and together with (28), this yields

$$|\hat{p}_1^{(1)} - \hat{p}_1^{(2)}| \le c(\kappa)\left(\|c_s^{(1)} - c_s^{(2)}\|_{W_r^{2-1/r}(Y)} + |C^{\mathcal{V}(1)} - C^{\mathcal{V}(2)}| + |\nabla_x V^{(1)} - \nabla_x V^{(2)}| + |P^{(1)} - P^{(2)}|\right).$$

Taking $t_j \in I$, $j = 1, 2$, and $f^{(j)} = f(t_j)$ for $f \in \{v, p, C^{\mathcal{V}}, c_s, \phi, V, P\}$ and dividing all estimates by $|t_1 - t_2|^\alpha$ finishes the proof. ☐

Remark 5.6. *The proof of Lemma 5.5 shows, that the operator $\mathcal{S}_1 : (\phi, c_s) \mapsto (v, p)$ is continuous.*

5.2 The Elasticity Equation and the Operator $\mathcal{S}_2$

In this section, we consider the elasticity equation (8), (9), (10). For the boundary condition $u = b$ on $\tilde{\Gamma}$ we assume throughout this section that b is the trace of a Y–periodic function $\bar{u} \in [W_r^2(Q_s)]^3$, with some $2 \le r < \infty$. Inserting $z = u - \bar{u}$ in (8), we get

$$-\operatorname{div}\sigma(z) = \operatorname{div}\sigma(\bar{u}) \;\text{ in } Q_s, \quad \sigma(z)n = g - \sigma(\bar{u})n \;\text{ on } \Gamma, \quad z = 0 \;\text{ on } \tilde{\Gamma}, \quad z \text{ is } Y-\text{periodic}, \tag{29}$$

where $g = 2\eta\, e(v)n - pn$. In order to derive a weak formulation of the problem, we assume for the moment that all functions are smooth. Let w be Y–periodic with $w|_{\tilde{\Gamma}} = 0$. We take the $\mathbb{R}^3$-scalar product of (29) with w, integrate over Q_s, integrate by parts and get due to the boundary conditions :

$$\int_{Q_s} \sigma(z) : e(w)\,\mathrm{d}y = -\int_{Q_s} \sigma(\bar{u}) : e(w)\,\mathrm{d}y + \int_\Gamma g \cdot w\,\mathrm{d}a.$$

Denote

$$a(z,w) := \int_{Q_s} \sigma(z) : e(w) \, \mathrm{d}y, \qquad \ell(w) := -\int_{Q_s} \sigma(\bar{u}) : e(w) \, \mathrm{d}y + \int_{\Gamma} g \cdot w \, \mathrm{d}a.$$

Then, for $2 \leq r < \infty$, $g \in \left(W_r^{1-1/r}(\Gamma)\right)'$ and $z \in [W_r^1(Q_s)]^3$, the functionals $a(z,\cdot)$ and $l(\cdot)$ are elements of $\left([W_r^1(Q_s)]^3\right)'$. We introduce the space

$$X = \{v \in [W_r^1(Q_s)]^3 \mid v|_{\bar{\Gamma}} = 0, v \text{ is } Y-\text{periodic}\}$$

and state the **weak formulation of the problem** (29):

$$\textit{Find } z \in X \textit{ such that } a(z,w) = \ell(w), \textit{ for all } w \in X. \tag{30}$$

For $r = 2$, the following version of Korn's inequality holds true:

Proposition 5.7. *Let $Y = [0,1]^2$. Every $z \in X$ satisfies*

$$\int_{Q_s} e(z) : e(z) \, \mathrm{d}y \geq \frac{c}{(1 + \|\phi\|_{L_\infty(Y)})^2 (1 + \|D\phi\|_{L_\infty(Y)})^4} \|z\|^2_{H^1(Q_s)}, \tag{31}$$

where the constant c is independent of ϕ.

Proof. Let $z \in X$. We extend z by zero for $y_3 < 0$. Denote by $R = h_A \max_{t \in I, y \in Y} |\phi(t,x)|$ a time independent upper bound for the thickness of $Q_s(t)$ in y_3-direction. Define $\hat{Q}_s = Y \times [0,R]$ and the transformation

$$\Psi_s(t) : \hat{Q}_s \to \tilde{Q}_s(t) : (\hat{y}_1, \hat{y}_2, \hat{y}_3) \mapsto (\hat{y}_1, \hat{y}_2, \hat{y}_3 + h_A \phi(t, y_1, y_2) - R), \tag{32}$$

(compare the transformation (16)), where $\tilde{Q}_s$ is the range of $\hat{Q}_s$ under Ψ_s ($\tilde{Q}_s$ is slightly bigger than Q_s). Due to the previous definitions we have $\|z\|_{H^1(\tilde{Q}_s)} = \|z\|_{H^1(Q_s)}$. Furthermore it is

$$\begin{aligned} \|\nabla z\|_{L_2(Q_s)} &\leq C \left(1 + \|D\phi\|_{L_\infty(Y)}\right) \|\nabla(z \circ \Psi_s)\|_{L_2(\hat{Q}_s)}, \\ \|e(z \circ \Psi_s)\|_{L_2(\hat{Q}_s)} &\leq C \left(1 + \|D\phi\|_{L_\infty(Y)}\right) \|e(z)\|_{L_2(Q_s)}. \end{aligned}$$

Denote $\hat{z} = z \circ \Psi_s$. For $\hat{z}$ we prove the First Korn inequality on $\hat{Q}_s$ by a combination of the proofs of [13], Chapter 2.5, Lemma 5.2 and [8], Theorem 3.4. We get

$$\|\nabla \hat{z}\|^2_{L_2(\hat{Q}_s)} \leq 2\|e(\hat{z})\|^2_{L_2(\hat{Q}_s)},$$

and consequently on Q_s:

$$\|\nabla z\|_{L_2(Q_s)} \leq c \left(1 + \|D\phi\|_{L_\infty(Y)}\right)^2 \|e(z)\|_{L_2(Q_s)}, \tag{33}$$

where the constant c is independent of ϕ. Then, the result follows from Poincaré's inequality with a constant depending only on the thickness of Q_s in y_3–direction (see e.g. [1], Theorem 6.30, pp.183-184):

$$\|z\|_{H^1(Q_s)} \leq (1 + h_A \|\phi\|_{L_\infty(Y)}) \|\nabla z\|_{L_2(Q_s)}.$$

□

The following theorem guaranties that the elastic problem has a unique solution:

Theorem 5.8. *Let $x \in S_0$, $t \in I$.*
1. Suppose that $2 \leq r < \infty$. Let $b \in [W_r^{1-1/r}(\tilde{\Gamma})]^3$ be the trace of a Y–periodic function $\bar{u} \in [W_r^1(Q_s)]^3$. Then (30) has a unique solution $z \in X$.
2. Suppose further that $\phi \in C^2(\bar{Y})$ with $\|\phi\|_{C^2(Y)} < \kappa$, for a constant $\kappa > 0$, and $b \in [W_r^{2-1/r}(\tilde{\Gamma})]^3$ is the

trace of a Y–periodic function $\bar{u} \in [W_r^2(Q_s)]^3$. Then, z is an element of $[W_r^2(Q_s)]^3$ and the displacement field $u = z + \bar{u} = \mathcal{S}_2(\phi, v, p)$ satisfies the a priori estimate

$$\|u(x,t)\|_{W_r^2(Q_s)} \le c(\kappa) \left(\|v(x,t)\|_{W_r^2(Q_{lK})} + \|p(x,t)\|_{W_r^1(Q_{lK})} + \|b(x,t)\|_{W_r^{2-1/r}(\tilde{\Gamma})} \right) \tag{34}$$

3. Let be $\hat{u} := u \circ \Psi_s$. It is $\hat{u} \in C^\alpha(I, W_r^2(\hat{Q}_s))$. The following estimate holds:

$$\|\hat{u}(x)\|_{C^\alpha(I,W_r^2(\hat{Q}_s))} \le c(\kappa) \Big(\|\hat{v}(x)\|_{C^\alpha(I,W_r^2(\hat{Q}_{lK}))} + \|\hat{p}(x)\|_{C^\alpha(I,W_r^1(\hat{Q}_{lK}))} + \|b(x)\|_{C^\alpha(I,W_r^{2-1/r}(\tilde{\Gamma}))} + \|\phi(x)\|_{C^\alpha(I,C^2(Y))} \Big)$$

Proof.

1. The linear operator $A : X \to X' : z \mapsto a(z, \cdot)$ is strictly monotone and hemicontinuous. Due to Proposition 5.7, it is coercive for $r = 2$. Then, Theorem 6.1 in [23] implies that A is also coercive for every real $r \ge 2$. We apply the Theorem of Browder and Minty (see e.g. [29], Theorem 26.A, p.557) and conclude that there exists a unique solution $z \in X$ of (30).

2. We localize the problem using a partition of unity $(\chi_i)_{i=1,\dots,M}$ as in the proof of Theorem 5.4. If $\operatorname{supp}(\chi_i) \cap \Gamma = \emptyset$, then it follows from the classical regularity results for the linear elastic problem with Dirichlet boundary conditions (see e.g. [25], Ch.III, §7, p.80, Theorem 7.1) that $\chi_i z \in [W_r^2(\Omega_i)]^3$. For $\operatorname{supp}(\chi_i) \cap \Gamma \neq \emptyset$, the same conclusion can be made using the corresponding results for Neumann boundary conditions (see e.g. [25], Ch.III, §7, p.83, Lemma 7.5). Analogously to the proof of Theorem 5.4, the estimate (34) can be derived using the L_r–estimates of Agmon, Douglis, Nirenberg (see [2], [3]) after a local transformation of our problems to domains with ϕ–independent boundary, but ϕ–dependent coefficients. In addition to the arguments of Theorem 5.4, note the following fact: After applying Theorem 10.5 of [3] to the localized and transformed elastic problems, the constant in the resulting estimate also depends on the constant of Korn's inequality. Thanks to Proposition 5.7, this constant can also be estimated in terms of κ.

3. From the definition (32) of Ψ_s, it follows that $\tilde{Q}_s = \Psi_s(\hat{Q}_s)$ is in general a strict superset of Q_s, while u is only defined as a function on Q_s. But $u = z + \bar{u}$ can be extended to $\tilde{Q}_s$ independently of ϕ in the following way: Set $z = 0$ for $y_3 < 0$ and extend the function b from (9) to a function $\bar{u} \in [W_r^2(Y \times [-R, R])]^3$. Then $\hat{u} = u \circ \Psi_s$ is well defined.

   The statement to prove follows as in the proof of Lemma 5.5.

□

5.3 The Microscopic Phase Field Equations and the Operator $\mathcal{S}_3$

In this section we discuss the solvability of the phase field version of the microscopic BCF-model (11) and (12). This system has to be solved for the phase field ϕ and the surface concentration c_s. These equations are valid for every $x \in S_0$ in $I \times Y$, where $I = [0, T]$ is a time interval and Y a periodicity cell. Furthermore, we have the initial conditions (13)

$$c_s(0, x, y) = c_{s,ini}(x, y), \qquad \phi(0, x, y) = \phi_{ini}(x, y),$$

and periodic boundary conditions for c_s and ϕ with respect to $(y_1, y_2) \in Y$. We consider Y–periodic test functions $w_1, w_2 \in L_2(I; H^1(Y))$, multiply equations (11) and (12) with w_1 and w_2 respectively, integrate by parts and get the following **weak formulation of the problem**:

Find Y–periodic c_s, $\phi \in L_2(I; H^1(Y))$ with $\partial_t c_s$, $\partial_t \phi \in L_2(I; H^1(Y)')$ such that the initial conditions (13) are satisfied and for every Y–periodic $w_1, w_2 \in L_2(I; H^1(Y))$ the following equations hold true:

$$\int_I \left(\langle \partial_t c_s, w_1 \rangle + \varrho_s h_A \langle \partial_t \phi, w_1 \rangle + \int_Y \left(D_s \nabla c_s \cdot \nabla w_1 + \left(\tfrac{c_s}{\tau_s} - \tfrac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} \right) w_1 \right) \mathrm{d}y \right) \mathrm{d}t = 0, \tag{35}$$

$$\int_I \left(\tau \xi^2 \langle \partial_t \phi, w_2 \rangle + \int_Y \left(\xi^2 \, \nabla \phi \cdot \nabla w_2 + (f'(\phi) + q(c_s, u, \phi)) \, w_2 \right) \mathrm{d}y \right) \mathrm{d}t = 0. \tag{36}$$

Here, $\langle\cdot,\cdot\rangle$ denotes the dual pairing on $H^1(Y)$. If $u \in [W_r^2(Q_s)]^3$, then we get for the trace of u on Γ: $(\sigma(u) : e(u)) \in W_{r/2}^{1-1/r}(Y)$, and $W_{r/2}^{1-1/r}(Y) \hookrightarrow L_2(Y)$ for $r \geq 5/2$. The equations above have the same structure as the microscopic problem in [6]. In addition to [6], we give a more detailed proof for the following solvability result:

Theorem 5.9. *Let be $c_{s,ini} \in L_2(Y)$, $\phi_{ini} \in L_2(Y)$ and $\hat{u} \in L_2(I, [W_r^2(\hat{Q}_s)]^3)$, for $r \geq 5/2$. Furthermore, suppose that the constants D_s, τ, ξ, h_A, ϱ_s, $\tau^{\mathcal{V}}$ and τ_s are positive. Then, the microscopic problem (35) and (36) at any fixed point $x \in S_0$ with given $C^{\mathcal{V}} = C^{\mathcal{V}}(\cdot, x) \in L_2(I)$ has a unique solution.*

Proof. The proof will be performed in several steps:

Step 1: Solve a linearized problem:
Consider, instead of (35), (36), the following 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 (13) are satisfied and for every $w_1, w_2 \in L_2(I; H^1_{\text{per}}(Y))$ the following equations hold true:

$$\int_I \left(\tau\xi^2 \langle \partial_t \phi, w_1 \rangle + \int_Y \xi^2 \nabla\phi \cdot \nabla w_1 \mathrm{d}y \right) \mathrm{d}t = -\int_{I\times Y} F(\hat{c}_s, \hat{\phi}) w_1 \,\mathrm{d}y\,\mathrm{d}t, \tag{37}$$

$$\int_I \left(\langle \partial_t c_s, w_2 \rangle + \int_Y \left(D_s \nabla c_s \cdot \nabla w_2 + \tfrac{1}{\tau_s} c_s w_2 \right) \mathrm{d}y \right) \mathrm{d}t = \int_I \left(\tfrac{1}{\tau^{\mathcal{V}}} \langle C^{\mathcal{V}}, w_2 \rangle - \varrho_s h_A \langle \partial_t \phi, w_2 \rangle \right) \mathrm{d}t, \tag{38}$$

with given $\hat{c}_s, \hat{\phi} \in L_2(I \times Y)$ and $F(c_s, \phi) = f'(\phi) + q(c_s, u, \phi)$.

Note, that F is Lipschitz continuous with respect to c_s and ϕ and grows at most linearily in c_s and ϕ, i.e.

$$|F(c_s, \phi)| \leq C\left(1 + |c_s| + |\phi|\right). \tag{39}$$

Therefore, if $\hat{c}_s, \hat{\phi} \in L_2(I \times Y)$, then it is also $F(\hat{c}_s, \hat{\phi}) \in L_2(I \times Y)$.

Equation (37) decouples from (38). It is, for given $\hat{c}_s$ and $\hat{\phi}$, a weak formulation of a linear heat equation for ϕ, independent of c_s. There exists a unique solution $\phi \in L_2(I, H^1(Y))$ of (37) with $\partial_t \phi \in L_2(I, H^1(Y)')$, see [20], p.379.

By the same reference, there is a unique solution $c_s \in L_2(I, H^1(Y))$ with $\partial_t c_s \in L_2(I, H^1(Y)')$ of (38), with the just found $\partial_t \phi$ on the righthand side.

Step 2: Estimates for the linearized problem:
Let $\hat{c}_{s,i}, \hat{\phi}_i \in L_2(I \times Y)$, $i = 1, 2$, and let $c_{s,i}, \phi_i$ be the corresponding solutions of (37), (38). Then the functions $\bar{c}_s := c_{s,1} - c_{s,2}$ and $\bar{\phi} := \phi_1 - \phi_2$ are solutions of

$$\int_I \tau\xi^2 \left(\langle \partial_t \bar{\phi}, w_1 \rangle + \int_Y \xi^2 \nabla\bar{\phi} \cdot \nabla w_1) \mathrm{d}y \right) \mathrm{d}t = -\int_{I\times Y} \left(F(\hat{c}_{s,1}, \hat{\phi}_1) - F(\hat{c}_{s,2}, \hat{\phi}_2) \right) w_1 \,\mathrm{d}y\,\mathrm{d}t, \tag{40}$$

$$\int_I \left(\langle \partial_t \bar{c}_s, w_2 \rangle + \int_Y \left(D_s \nabla \bar{c}_s \cdot \nabla w_2 + \tfrac{1}{\tau_s} \bar{c}_s w_2 \right) \mathrm{d}y \right) \mathrm{d}t = -\int_I \varrho_s h_A \langle \partial_t \bar{\phi}, w_2 \rangle \mathrm{d}t, \tag{41}$$

with $\bar{\phi}(0) = \bar{c}_s(0) = 0$. For $z \in \{\bar{c}_s, \bar{\phi}\}$ and $0 < t \leq T$, we have $\partial_t \|z(t)\|^2_{L_2(Y)} = 2\langle \partial_t z, z\rangle(t)$ and thus

$$\int_0^t \langle \partial_t z, z \rangle \mathrm{d}t = \frac{1}{2} \left(\|z(t)\|^2_{L_2(Y)} - \|z(0)\|^2_{L_2(Y)} \right) = \frac{1}{2} \|z(t)\|^2_{L_2(Y)}. \tag{42}$$

Let be $0 < t \leq T$ and $I_t = [0, t]$. Taking $w_1 = \chi_{I_t}(\phi_1 - \phi_2)$ in (40) and using the Lipschitz continuity of F, we get with (42) and Young's inequality (see e.g. [11], p.622)

$$\begin{aligned} \|(\phi_1 - \phi_2)(t)\|^2_{L_2(Y)} + \|\nabla(\phi_1 - \phi_2)\|^2_{L_2(I_t\times Y)} \leq C \Big(&\|\phi_1 - \phi_2\|^2_{L_2(I_t\times Y)} + \|\hat{c}_{s,1} - \hat{c}_{s,2}\|^2_{L_2(I_t\times Y)} \\ &+ \|\hat{\phi}_1 - \hat{\phi}_2\|^2_{L_2(I_t\times Y)} \Big). \end{aligned}$$

This estimate also holds, if the gradient term on the lefthand side is neglected. Gronwall's inequality (see e.g. [11], p.625) then implies

$$\|\phi_1 - \phi_2\|_{L_\infty(I,L_2(Y))} \leq C\left(\|\hat{c}_{s,1} - \hat{c}_{s,2}\|_{L_2(I\times Y)} + \|\hat{\phi}_1 - \hat{\phi}_2\|_{L_2(I\times Y)}\right). \tag{43}$$

Due to the continuous embedding $L_\infty(I, L_2(Y)) \hookrightarrow L_2(I \times Y)$, we also get

$$\|\phi_1 - \phi_2\|_{L_2(I,H^1(Y))} \leq C\left(\|\hat{c}_{s,1} - \hat{c}_{s,2}\|_{L_2(I\times Y)} + \|\hat{\phi}_1 - \hat{\phi}_2\|_{L_2(I\times Y)}\right),$$

and with (40)

$$\|\partial_t(\phi_1 - \phi_2)\|_{L_2(I,H^1(Y)')} \leq C\left(\|\hat{c}_{s,1} - \hat{c}_{s,2}\|_{L_2(I\times Y)} + \|\hat{\phi}_1 - \hat{\phi}_2\|_{L_2(I\times Y)}\right). \tag{44}$$

Setting $w_2 = \chi_{I_t}(c_{s,1} - c_{s,2})$ in (41), we get again with Young's inequality

$$\begin{aligned}\|(c_{s,1} - c_{s,2})(t)\|^2_{L_2(Y)} + \|c_{s,1} - c_{s,2}\|^2_{L_2(I_t,H^1(Y))} &\leq \left|\int_{I_t} \langle \partial_t(\phi_1 - \phi_2), c_{s,1} - c_{s,2}\rangle \mathrm{d}t\right| \\ &\leq \frac{1}{\varepsilon}\|\partial_t(\phi_1 - \phi_2)\|^2_{L_2(I_t,H^1(Y)')} + \varepsilon\|c_{s,1} - c_{s,2}\|^2_{L_2(I_t,H^1(Y))},\end{aligned}$$

which implies together with (44) and for $\varepsilon > 0$ small enough

$$\|c_{s,1} - c_{s,2}\|_{L_\infty(I,L_2(Y))} + \|c_{s,1} - c_{s,2}\|_{L_2(I,H^1(Y))} \leq C\left(\|\hat{c}_{s,1} - \hat{c}_{s,2}\|_{L_2(I\times Y)} + \|\hat{\phi}_1 - \hat{\phi}_2\|_{L_2(I\times Y)}\right). \tag{45}$$

An obvious consequence of the estimates (43) and (45) is

$$\|\phi_1 - \phi_2\|_{L_\infty(I,L_2(Y))} + \|c_{s,1} - c_{s,2}\|_{L_\infty(I,L_2(Y))} \leq C\left(\|\hat{c}_{s,1} - \hat{c}_{s,2}\|_{L_2(I\times Y)} + \|\hat{\phi}_1 - \hat{\phi}_2\|_{L_2(I\times Y)}\right). \tag{46}$$

Step 3: Solve the original semi–linear problem using a fixed point argument: We define the solution operator

$$\mathcal{T}\colon [L_\infty(I, L_2(Y))]^2 \to [L_\infty(I, L_2(Y))]^2\colon (\hat{c}_s, \hat{\phi}) \mapsto (c_s, \phi),$$

which maps given $(\hat{c}_s, \hat{\phi})$ to the corresponding solutions of (37), (38). Note, that every function $w \in L_\infty(I, L_2(Y))$ satisfies

$$\|w\|_{L_2(I,L_2(Y))} \leq T^{1/2}\|w\|_{L_\infty(I,L_2(Y))}.$$

This implies, together with estimate (46):

$$\|\mathcal{T}(\hat{c}_{s,1} - \hat{c}_{s,2}, \hat{\phi}_1 - \hat{\phi}_2)\|_{L_\infty(I,L_2(Y))} \leq CT^{1/2}\|(\hat{c}_{s,1} - \hat{c}_{s,2}, \hat{\phi}_1 - \hat{\phi}_2)\|_{L_\infty(I,L_2(Y))}.$$

Choose $0 < T_1 \leq T$ small enough, such that $CT_1^{1/2} < 1$. Then, restricted to the time interval $I_{T_1} := [0, T_1]$, the operator

$$\mathcal{T}\colon [L_\infty(I_{T_1}, L_2(Y))]^2 \to [L_\infty(I_{T_1}, L_2(Y))]^2$$

is a contraction. Banach's fixed point theorem proves the existence of a solution (c_s, ϕ) of (35), (36) on the possibly reduced time interval $[0, T_1]$. Since the choice of T_1 is independent of the solution (c_s, ϕ) and its intial data $(c_{s,ini}, \phi_{ini})$, finitely many repetitions of this arguments, with $(c_s, \phi)(T_1)$ replacing the initial data, prove the existence of a solution on the whole time interval $[0, T]$. Uniqueness of that solution follows from (46) and Gronwall's inequality. □

In the proofs of existence and regularity of solutions of the Stokes problem and the elastic equation, we assumed higher regularity for both ϕ and c_s, namely $\phi, c_s \in C^2(Y)$. In fact, ϕ and c_s are, under certain conditions, more regular as stated above, namely:

Theorem 5.10. *Assume that all conditions of Theorem 5.9 are satisfied. Suppose in addition that* $c_{s,ini}, \phi_{ini} \in C^{2+2\alpha}(Y)$, $C^{\mathcal{V}} \in C^\alpha(I)$ *and* $\hat{u} \in C^\alpha(I, [W^2_r(\hat{Q}_s)]^3)$, *for* $r > \frac{5}{1-2\alpha}$, $0 < \alpha < \frac{1}{4}$. *Then* $(\phi, c_s) = \mathcal{S}_3(\hat{u})$ *is an element of* $\left[C^{1+\alpha,2+2\alpha}(I \times Y)\right]^2$.

Proof. We get for the trace of u on Γ that $\sigma(u) : e(u) \in C^{2\alpha}(Y)$, if $r > 5/(1-2\alpha)$ and $u \in W^2_r(Q_s)$. The following proof uses regularity results for the linear heat equation with Dirichlet boundary conditions, namely Theorem 9.1 of Ch.IV in [15] for Sobolev spaces and Theorem 5.1.15 of Ch.5 in [16] for Hölder spaces. Therefore, we reformulate the problem:

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain such that $\bar{Y} \subset \Omega$ with $C^{2+2\alpha}$–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, consider the functions $\chi\phi$ and χc_s. If ϕ and c_s solve (35) and (36) on $I \times Y$, then $\chi\phi$ and χc_s are weak solutions of

$$\tau\xi^2\partial_t(\chi\phi) - \xi^2\Delta(\chi\phi) = -\chi\left(f'(\phi) + q(c_s,u,\phi)\right) - \xi^2\left(\phi\Delta\chi + 2\nabla\chi\nabla\phi\right), \tag{47}$$

$$\partial_t(\chi c_s) - D_s\Delta(\chi c_s) = \chi\left(\frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{c_s}{\tau_s} - \varrho_s h_A \partial_t\phi\right) - D_s\left(c_s\Delta\chi + 2\nabla\chi\nabla c_s\right) \tag{48}$$

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

$$\chi c_s(0,y) = \chi c_{s,ini}(y), \qquad \chi\phi(0,y) = \chi\phi_{ini}(y),$$

where $c_{s,ini}, \phi_{ini}$ are also extended periodically to Ω. From $c_s, \phi \in L_2(I, H^1(\Omega))$ it follows, that the righthand side of (47) is in $L_2(I \times \Omega)$, since f' and q grow at most linearily (This argument is also true if L_2 is replaced by any L_r, $1 \le r \le \infty$). Then, the application of Theorem 9.1 of Ch.IV in [15] yields

$$\chi\phi \in W_2^{1,2}(I \times \Omega), \quad \text{ and therefore } \quad \phi \in W_2^{1,2}(I \times Y).$$

Note, that this implies $\partial_t\phi \in L_2(I \times Y)$. Theorem 9.1 of Ch.IV in [15] can now be applied to equation (48) and this yields

$$c_s \in W_2^{1,2}(I \times Y), \quad \text{ and thus } \quad c_s, \phi \in W_4^{0,1}(I \times Y),$$

due to the embedding $W_2^{1,2}(I \times Y) \hookrightarrow W_4^{0,1}(I \times Y)$, see [9], Thm. 2.2.2, p.22. Repetition of the same argument for both equations with 4 as the order of integration instead of 2 implies $c_s, \phi \in W_4^{1,2}(I \times Y)$, and thus $c_s, \phi \in W_s^{0,1}(I \times Y)$, for all $s \ge 1$. Another application of Theorem 9.1 of Ch.IV in [15] yields

$$c_s, \phi \in W_s^{1,2}(I \times Y)$$

for any $1 < s < +\infty$. Next, for $0 < \lambda < 1$, we have the interpolation $W_s^{1,2}(I \times Y) \hookrightarrow W_s^\lambda(I, W_s^{2(1-\lambda)}(Y))$, see [9], Corollary 2.2.6, p.23. The embeddings

$$W_s^\lambda(I, W_s^{2(1-\lambda)}(Y)) \hookrightarrow C^\alpha(I, W_s^{2(1-\lambda)}(Y)), \qquad W_s^{2(1-\lambda)}(Y) \hookrightarrow C^{1+2\alpha}(Y)$$

are valid for $\lambda - \frac{1}{s} > \alpha$ and for $2(1-\lambda) - \frac{2}{s} > 1 + 2\alpha$. It follows that

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

for $s > \frac{4}{1-4\alpha}$, $0 < \alpha < \frac{1}{4}$. Thus $c_s, \phi \in C^\alpha(I, C^{1+2\alpha}(Y)$ which implies, that the righthand side of (47) is an element of $C^{\alpha,2\alpha}(I \times Y)$, which makes Theorem 5.1.15 of Ch.5 in [16] applicable – first to (47) and afterwards to (48). Finally, this proves

$$c_s, \phi \in C^{1+\alpha,2+2\alpha}(I \times Y).$$

$\square$

6 Conclusion

- In this paper, a two scale model for liquid phase epitaxy with elasticity is presented.
- The coupling of the microscopic and the macroscopic equations is described by an iterative procedure.
- The macroscopic equations do not change in comparison with the corresponding model without elasticity but more regularity assumptions are needed.
- We focus on the microscopic equations and study their solvability in appropriate function spaces. As main results we prove the existence and uniqueness of solutions of the three single parts of the microscopic problem. The composition of the corresponding solution operators maps a suitable function space into itself.

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Christof Eck
We mourn the death of Prof. Dr. Christof Eck. He passed away on September 14th, 2011.

Michael Kutter
Pfaffenwaldring 57
70569 Stuttgart
Germany
E-Mail: Michael.Kutter@mathematik.uni-stuttgart.de
WWW: http://www.mathematik.uni-stuttgart.de/fak8/ians/mitarbeiter/kutter.html

Anna-Margarete Sändig
Pfaffenwaldring 57
70569 Stuttgart
Germany
E-Mail: Anna.Saendig@mathematik.uni-stuttgart.de

Christian Rohde
Pfaffenwaldring 57
70569 Stuttgart
Germany
E-Mail: Christian.Rohde@mathematik.uni-stuttgart.de

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