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Well-Posedness of a Two Scale Model for Liquid Phase Epitaxy with Elasticity

Michael Kutter* Christian Rohde* Anna-Margarete Sändig*

Abstract

Epitaxy, a special form of crystal growth, is a technically relevant process for the production of thin films and layers. It can generate microstructures of different morphologies, such as steps, spirals or pyramids. These microstructures are influenced by elastic effects in the epitaxial layer. There are different epitaxial techniques, one being liquid phase epitaxy. Thereby, single particles are deposited out of a supersaturated liquid solution on a substrate where they contribute to the growth process.

This article studies a two scale model including elasticity, introduced in [Ch. Eck, H. Emmerich. Homogenization and two-scale models for liquid phase epitaxy. *Eur. Phys. J. Special Topics* **177**, 5–21 (2009)] and extended in [Ch. Eck, H. Emmerich. Liquid-phase epitaxy with elasticity. *Preprint 197*, DFG SPP 1095 (2006)]. 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 Burton-Cabrera-Frank model for the evolution of the epitaxial layer, a Stokes system for the fluid flow near the layer and an elasticity system for the elastic deformation of the solid film. Suitable conditions couple the single parts of the model.

As the main result, existence and uniqueness of a solution is proven in suitable function spaces. Furthermore, an iterative solving procedure is proposed, which reflects on the one hand the strategy of the proof of the main result via fixed point arguments and, on the other hand, can be the basis for a numerical algorithm.

Keywords: Liquid phase epitaxy with elasticity, two scale model, phase field models, existence and regularity of solutions

1 Introduction

In liquid phase epitaxy, [28], single particles of a certain substance (e.g. silicon) are deposited out of a supersaturated liquid solution on a substrate. The substrate is made of the same material (homoepitaxy) or a similar but different one (heteroepitaxy). The particles (at that stage called *adatoms*) can move on its surface, driven by diffusion, until a crystal growth process can be observed and a thin epitaxial film forms: one monomolecular layer after another. This technique is often used for the production of semiconductor devices, such as solar cells, integrated circuits, lasers and light emitting diodes. Experiments have shown, e.g. [5], that the layer usually generates microstructures of different morphologies. Especially in the case of heteroepitaxy, their development is influenced by elastic effects, which occur due to different crystal structures of the materials of substrate and layer, [12].

There are different approaches to model liquid phase epitaxy. Purely continuum models, [19, 30, 32], describe the height of the solid film by nonlinear partial differential equations and do not resolve the stepped structure of the surface. Purely discrete models describe the movement of each particle and their interactions by kinetic Monte Carlo methods, [26]. The major disadvantage of these models is, that they are only applicable at very small length scales. Furthermore, there are semi-discrete models, based on the work of Burton, Cabrera and Frank (BCF model), [3]. The diffusion process along the surface is

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described by continuum equations, while in perpendicular direction, the monomolecular steps are resolved in a discrete way. As a variant of the BCF model, phase field models have been established, [8, 15, 18, 22]. Based on the ideas of diffuse interface models for phase transitions in solidification processes, [4], the steps from one monomolecular layer to another are smoothed, where the thickness of the smooth transition region is controlled by a small parameter. In fact, in this context, the edges of the monomolecular steps are considered as phase transitions, whereby a "phase" does not indicate the state of aggregation (solid/liquid), but the thickness of the epitaxial layer, measured by the number of monomolecular layers. Consequently, not only two but multiple phases are involved in the process. These phase field models, in contrast to "sharp step" BCF models, are easier to handle from the analytical as well as from the numerical point of view.

A huge challenge for the simulation of an epitaxial process is the calculation of the microstructure. A numerical grid has to resolve it, which makes computations on a technically relevant length scale very expensive or even impossible. Homogenization leads to the formulation of two scale models which paves the way for an efficient implementation. For liquid phase epitaxy, such a model has been derived in [8]. The model describes the transport process in the liquid solution by continuum equations and the epitaxial growth with a phase field version of the BCF model. The homogenization here leads to a macroscopic domain, which is fully occupied by the liquid solution, and for every point on the substrate, microscopic BCF problems have to be solved for the calculation of the microstructure. Coupling conditions, which act as boundary conditions on the macroscopic scale, model the interaction between the liquid solution and the epitaxial layer. The well-posedness of the model has been proven and the formal derivation of the two scale model was justified rigorously, see [8]. The model of [8] was further developed in [9] and [10], where elastic effects are included. The main difference to [8] is, that the microscopic cell problems consist not only of BCF models, but also of equations for the description of the elastic effects and the fluid flow near the surface of the layer. The consequences on the mathematical analysis and numerics for the model are tremendous. While the model without elasticity consists essentially of semi-linear partial differential equations, the extended microscopic problems are fully nonlinear.

In this paper, the well-posedness of the two scale model with elasticity, proposed in [10], is proven. Section 2 presents the model and shortly explains the derivation of the two scale formulation. In section 3, the model is investigated from the analytical point of view. The main result of the section and the paper is the existence and uniqueness of solutions of the fully coupled model problem, see Theorem 3.1. Section 4 recapitulates the strategy of the proof of the main result and developes an iterative solving procedure, which can be used as a basis for a numerical algorithm. Convergence of the iteration is proven.

The paper is based on the PhD thesis [16].

2 The Mathematical Model

In this section, the model from [10] is introduced. First, the non-homogenized model is presented in sections 2.1 and 2.2, and second, the two scale model in section 2.3. The latter is derived from the non-homogenized model using homogenization techniques. The ansatz for the derivation is explained in section 2.3, but for technical details, the reader is referred to [10].

2.1 Physical Model

The physical situation is the following: Consider a time interval $I = [0, T]$ and a domain $Q \subset \mathbb{R}^3$ which has the form of a container, see Figure 1, and is filled with a liquid solution that contains the particles from which an epitaxial layer grows on a substrate. The contact to the substrate is at the bottom of Q, which is denoted by

$$S_0 := \{x \in \overline{Q} \mid x_3 = 0\}.$$

The solid film grows on S_0, the time dependent domain occupied by that film is denoted by $Q^S = Q^S(t)$. The liquid domain is $Q^L(t) = Q \setminus \overline{Q^S(t)}$. It is assumed that the interface S between Q^S (solid material) and Q^L (liquid solution) can be represented as the graph of a function $h\colon S_0 \to [0, \infty)$ over S_0:

$$S(t) = \{x \in Q \mid x_3 = h(x_1, x_2, t)\},$$

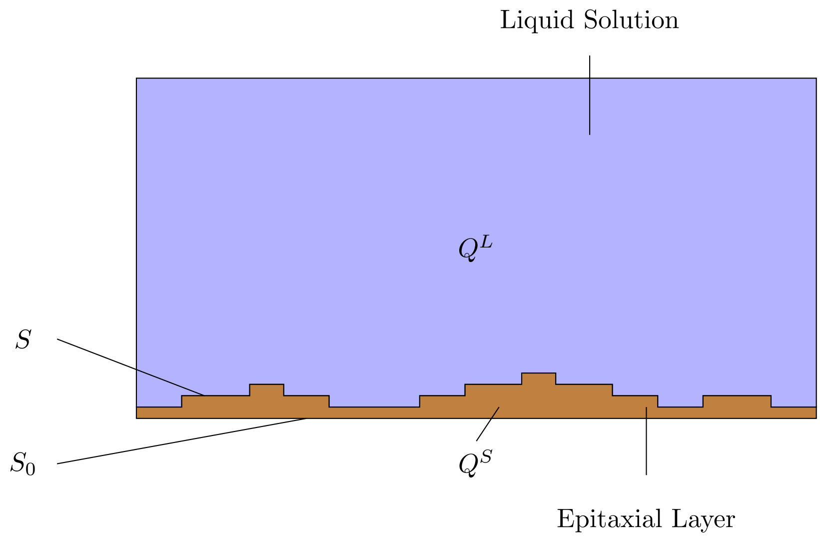
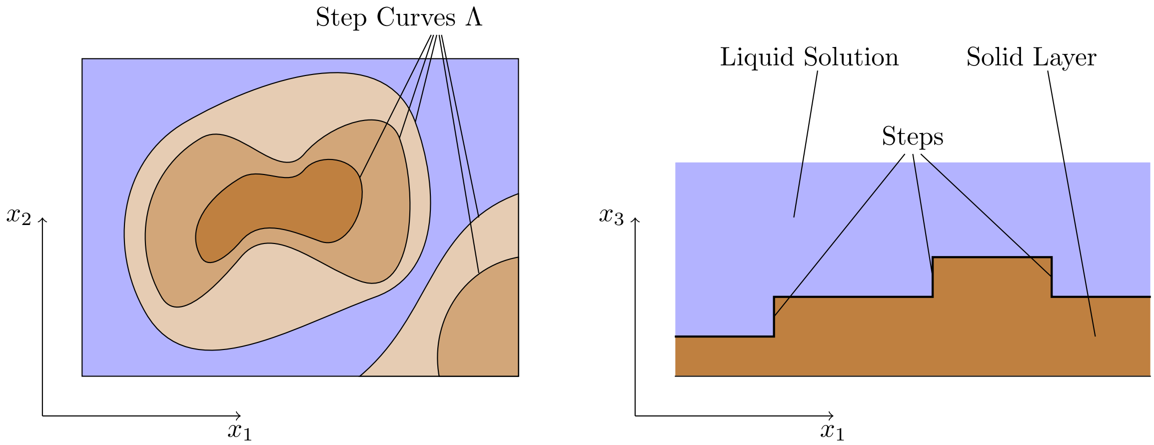


Figure 1: Liquid Phase Epitaxy.

and therefore

$$Q^S(t) = \{x \in Q \mid x_3 < h(x_1, x_2, t)\},$$
$$Q^L(t) = \{x \in Q \mid x_3 > h(x_1, x_2, t)\}.$$

The process is modeled as step by step growth, see Figure 2(b). This means, that the solid film grows one monomolecular layer after another. The description of the steps can be reduced to a two dimensional problem by considering a step as a curve in the two dimensional domain S_0, see Figure 2(a). The union of these curves is denoted by $\Lambda = \Lambda(t)$.



(a) Top View.

(b) Cross Section.

Figure 2: Step by Step Growth.

Thus, the model contains two different types of free boundaries: One is the interface $S = S(t)$ between the liquid solution and solid layer, the other consists of the step curves $\Lambda = \Lambda(t)$ which are introduced above.

The processes to be described are:

i) Volumic transport of the particles in the liquid solution, driven by convection and diffusion.

ii) Adsorption of particles to the surface. At that stage, the particles are called *adatoms*.

iii) Surface diffusion: Adatoms move on the surface, driven by diffusion, until they desorb into the liquid solution or they reach a step and incorporate into the layer.

iv) Elastic effects in the layer.

Summarizing, there are three different types of processes: in the liquid, in the solid and on the interface. In order to model these effects, partial differential equations are formulated in each of these three parts and suitable coupling conditions are derived. Hereby, the coupling takes place at the interface S. More precisely, the model is composed of the following parts:

- In $I \times Q^L$, a **Navier-Stokes system** has to be solved for the fluid flow and the pressure, and a **convection-diffusion equation** for the transport of particles in the liquid solution,

$$\begin{aligned} \operatorname{div} v &= 0, \\ \partial_t v + (v \cdot \nabla) v - \eta \Delta v + \nabla p &= 0, \end{aligned} \tag{2.1}$$

$$\partial_t c^{\mathcal{V}} + v \cdot \nabla c^{\mathcal{V}} - D^{\mathcal{V}} \Delta c^{\mathcal{V}} = 0, \tag{2.2}$$

  where v is the fluid velocity, p the pressure, $c^{\mathcal{V}}$ the mass specific volume concentration of particles in the liquid solution ("$\mathcal{V}$" stands for "volume"), η the viscosity of the liquid and $D^{\mathcal{V}}$ the diffusion constant of the volumic diffusion process.

  Boundary conditions are

$$D^{\mathcal{V}} \frac{\partial c^{\mathcal{V}}}{\partial n} = J_S^{-1}(1 - c^{\mathcal{V}}) \left(\frac{c_s}{\tau_s} - \frac{c^{\mathcal{V}}}{\tau^{\mathcal{V}}} \right), \qquad v = J_S^{-1} \left(\frac{1}{\varrho^{\mathcal{V}}} - \frac{1}{\varrho_E} \right) \left(\frac{c^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{c_s}{\tau_s} \right) n_L, \quad \text{on } S, \tag{2.3}$$

$$D^{\mathcal{V}} \frac{\partial c^{\mathcal{V}}}{\partial n} = 0, \qquad v = 0, \qquad \text{on } \partial Q^L \setminus S, \tag{2.4}$$

  where c_s is the surface concentration of adatoms (see also the BCF-model for the evolution of the interface), $J_S = \sqrt{1 + |\nabla h|^2}$ is the density of the surface measure of S, parameterized over S_0, $\varrho^{\mathcal{V}}$ and ϱ_E are the densities of the liquid solution and the solid layer respectively, τ_s and $\tau^{\mathcal{V}}$ describe the rates of adsorption and desorption of adatoms from and to the liquid solution, and $n_L = \frac{1}{\sqrt{1+|\nabla h|^2}}((\nabla h)^\top, -1)^\top$ is the outer normal on ∂Q^L at S. The coupling conditions (2.3) are derived under the assumption of conservation of the total mass and of the mass of adatoms, see [10], pp. 4-5.

  Furthermore, there are initial conditions

$$v(\cdot, 0) = v_{ini}, \qquad c^{\mathcal{V}}(\cdot, 0) = c^{\mathcal{V}}_{ini}. \tag{2.5}$$

- For the description of the elastic effects, there is for each $t \in I$ a quasi-stationary **elasticity equation**

$$-\operatorname{div} \sigma(u) = 0, \qquad \text{in } Q^S, \tag{2.6}$$

  with displacement field u, stress tensor $\sigma(u)$, given by the linear Hooke law $\sigma(u) = \mathbf{C} e(u)$ with linearized strain tensor $e(u) = \frac{1}{2}(\nabla u + (\nabla u)^\top)$ and elastic material tensor $\mathbf{C}$. The elastic deformation is driven by a misfit between substrate and epitaxial layer, which occurs due to different crystal structures. A simple model therefor is a prescribed misfit displacement b, that leads to the boundary condition

$$u = b, \qquad \text{on } S_0. \tag{2.7}$$

  The coupling to the liquid solution is derived from the equilibrium of normal stresses

$$\sigma(u) n_S - \eta\, e(v)\, n_S + p n_S = 0, \qquad \text{on } S, \tag{2.8}$$

where $n_S = \frac{1}{\sqrt{1+|\nabla h|^2}}(-(\nabla h)^\top, 1)^\top$ is the outer normal on ∂Q^S at S. The boundary condition

$$\sigma(u)n = 0, \qquad \text{on } \partial Q^S \setminus (S_0 \cup S), \tag{2.9}$$

completes this part of the model.

- The evolution of the epitaxial layer is described by a **Burton-Cabrera-Frank (BCF) model**

$$\partial_t c_s = D_s \Delta c_s + \frac{c^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{c_s}{\tau_s}, \qquad t \in I, x \in S_0 \setminus \Lambda(t), \tag{2.10}$$

$$c_s = c_{\text{eq}} \left(1 + \frac{\kappa\gamma}{\varrho_s R \mathcal{T}}\right) + \frac{h_A}{2R\mathcal{T}} \sigma(u) : e(u), \qquad t \in I, x \in \Lambda(t), \tag{2.11}$$

$$v_\Lambda = \frac{D_s}{\varrho_s} \left[\frac{\partial c_s}{\partial n}\right], \qquad t \in I, x \in \Lambda(t). \tag{2.12}$$

Here c_s is the surface concentration of adatoms ("s" stands for "surface"), measured by the mass of adatoms per unit area, $\varrho_s = \frac{m_A}{A_A}$ with mass m_A and area A_A of one adatom is the surface density of adatoms, D_s the surface diffusion constant, c_{eq} the equilibrium surface concentration at the monomolecular step, κ the curvature of the step, γ the step stiffness, $R = \frac{k_B}{m_A}$ the gas constant with Boltzmann constant k_B, $\mathcal{T}$ the temperature, h_A the height of one step and v_Λ the velocity of the steps. The bracket $\left[\frac{\partial c_s}{\partial n}\right]$ denotes the difference of the normal derivatives on both sides of the curves Λ,

$$\left[\frac{\partial c_s}{\partial n}\right] = \nabla c_s^+ \cdot n^+ + \nabla c_s^- \cdot n^-,$$

where $c_s^\pm = \lim_{r\to 0} c_s(x + rn^\pm)$ for $x \in \Lambda$ with normal vector $n^+ = n$ on Λ and $n^- = -n$. This part of the model is formulated on the surface S_0 and, therefore, the spatial derivatives have to be understood as two dimensional (with respect to x_1 and x_2).

Finally, there are the boundary and initial conditions

$$D_s \frac{\partial c_s}{\partial n} = 0, \quad \text{on } I \times \partial S_0, \qquad c_s(\cdot, 0) = c_{s,ini}, \quad \Lambda(0) = \Lambda_{ini}. \tag{2.13}$$

- The **evolution of the interface** S is described by

$$\partial_t h = \frac{1}{\varrho_E} \left(\frac{c^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{c_s}{\tau_s}\right), \tag{2.14}$$

with $h(\cdot, 0) = h_{ini}$.

In contradiction to the concept of step by step growth, with sharp step edges, the interface S is considered as smooth surface in the context of the fluid flow and elasticity problems. The authors in [10] justify this by the fact, that the equations there are continuum-scale equations and that their scale is much larger than that of the monomolecular layers.
Furthermore, for the analysis as well as for the numerics, a smooth transition from step to step is more convenient than the modeling by sharp steps. An approach therefor is the formulation of a phase field approximation of the BCF model, which is presented in the next section.

2.2 Phase Field Approximation

Introduce a phase field function $\phi\colon S_0 \to [0, \infty)$ which describes the height of the epitaxial film over a point on S_0 by the number of monomolecular layers, see Figure 3. The use of the notion of "phase" and "phase field" expresses the mathematical similarity to diffuse interface models for solidifaction processes, see [4].
A "phase" here does not indicate the state of aggregation (solid/liquid), but the thickness of the epitaxial layer, measured by the number of monomolecular layers, and a step is interpreted as a phase transition. So, multiple phases occur in the process. The natural values of ϕ would be the nonnegative integers, but

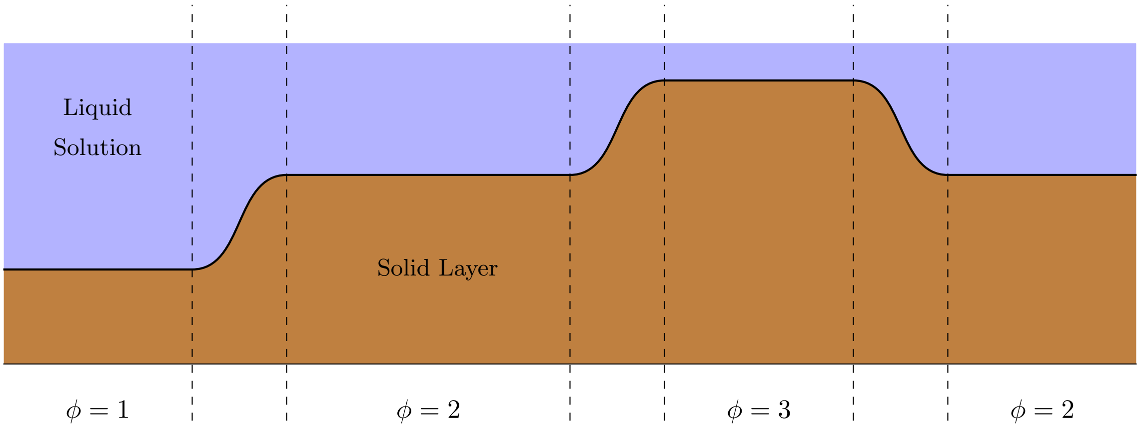


Figure 3: The Phase Field.

ϕ is allowed to take real values in a neighborhood of a step which enables a smooth transition from step to step.
The BCF model (2.10) - (2.13) is replaced by a phase field approximation. It is derived from the free energy functional

$$\mathcal{F}(\phi) = \int_{S_0} \Big[\frac{c_{\text{eq}}\gamma\beta}{\varrho_s} \left(\frac{\xi}{2} |\nabla\phi|^2 + \frac{1}{\xi} f(\phi) \right) - R\mathcal{T}(c_s - c_{\text{eq}})\, g_1(\phi) + \frac{h_A}{2} \sigma(u) : e(u)\, g_2(\phi) \Big] \mathrm{d}x,$$

with a multi-well potential f which has its minima at integer values, for example $f(\phi) = -\cos(2\pi\phi)$. The parameter ξ describes the thickness of the smooth transition regions. In [10] the functions g_1 and g_2 are chosen as $g_1(\phi) = g_2(\phi) = \phi$. Following the suggestions of [15] (where a model without elastic effects is discussed), another possible choice is

$$g_1(\phi) = \frac{1}{2} \left(\phi - \frac{\sin(2\pi\phi)}{2\pi} \right), \tag{2.15}$$

which keeps the minima of the corresponding term in $\mathcal{F}$ with respect to ϕ at integer values $\phi \in \mathbb{N}_0$. Another possible choice for g_2 is discussed at the end of this section.
The parameter β is given by

$$\beta^{-1} = \int_{-\infty}^{+\infty} \left((\varphi'(x))^2 + f(\varphi(x)) \right) \mathrm{d}x,$$

where φ is the solution of

$$-\varphi''(x) + f'(\varphi(x)) = 0, \quad \lim_{x\to-\infty} \varphi(x) = 0, \quad \lim_{x\to+\infty} \varphi(x) = 1, \quad \varphi(0) = \frac{1}{2}.$$

As in [4], the ansatz $\alpha\partial_t\phi = -D_\phi\mathcal{F}(\phi)$, where $\alpha > 0$ is a relaxation parameter and $D_\phi\mathcal{F}$ the Gâteaux derivative of $\mathcal{F}$ with respect to ϕ, leads to

$$\alpha\partial_t\phi = \frac{c_{\text{eq}}\gamma\beta}{\varrho_s} \left(\xi\Delta\phi - \frac{1}{\xi} f'(\phi) \right) + R\mathcal{T}(c_s - c_{\text{eq}})\, g_1'(\phi) - \frac{h_A}{2} \sigma(u) : e(u)\, g_2'(\phi)$$

in $I \times S_0$. After rescaling, this results in the phase field equation

$$\tau\xi^2\partial_t\phi - \xi^2\Delta\phi + f'(\phi) + q(\phi, c_s, u) = 0, \qquad \text{in } I \times S_0, \tag{2.16}$$

with $\tau = \frac{\alpha\varrho_s}{c_{\text{eq}}\gamma\beta}$ and

$$q(\phi, c_s, u) = \frac{\xi R\mathcal{T}\varrho_s}{c_{\text{eq}}\gamma\beta} (c_{\text{eq}} - c_s)\, g_1'(\phi) + \frac{\xi h_A \varrho_s}{2c_{\text{eq}}\gamma\beta} \sigma(u) : e(u)\, g_2'(\phi). \tag{2.17}$$

With the choice of [10], the functions g_1' and g_2' are constant $g_1'(\phi) = g_2'(\phi) = 1$, while from (2.15), the derivative g_1' acts like a switch: The corresponding term is only nonzero, if $\phi \notin \mathbb{N}_0$, which is only in the transition regions in the neighborhood of a step. For the analysis in section 3, both choices are allowed. ϕ is endowed with an initial condition

$$\phi(\cdot, 0) = \phi_{ini}, \tag{2.18}$$

and a boundary condition

$$\frac{\partial \phi}{\partial n} = 0, \qquad \text{on } I \times \partial S_0. \tag{2.19}$$

The surface diffusion equation (2.10) is modified to

$$\partial_t c_s + \varrho_s \partial_t \phi - D_s \Delta c_s = \frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{c_s}{\tau_s}, \tag{2.20}$$

compare the corresponding equation in [4]. The additional term $\varrho_s \partial_t \phi$ describes the conservation of adatoms.
The BCF model (2.10) - (2.12) can be interpreted as a sharp interface limit of (2.16), (2.20), see [8, 13, 15].

2.3 Two Scale Model

The single processes during the growth of the epitaxial layer have completely different length scales. The smallest is that of a particle diameter, which is approximately the height h_A of one monomolecular layer, the largest is that of the continuum equations for the fluid flow and the typical size of the microstructure lies somewhere in between.

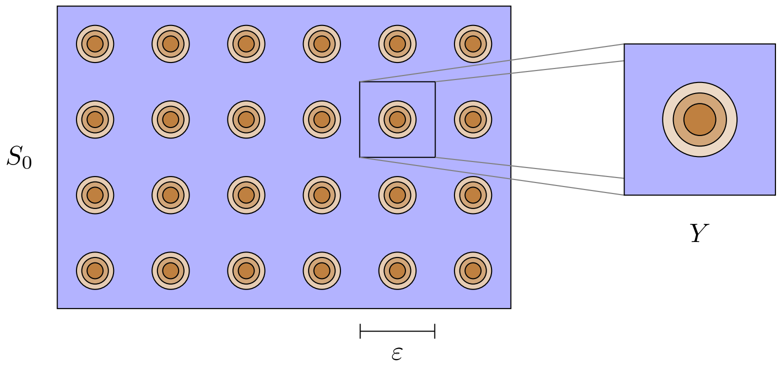


Figure 4: Periodic Homogenization in the x_1-x_2-Plane.

The main idea of the two scale formulation of the model is, to use different spatial variables for processes with different length scales. The model is derived by homogenization techniques with homogenization parameter ε. Here, ε represents the scale of the microstructure. In the following, the ansatz is explained and the resulting model is presented. For the technical details, see [10].
As ansatz it is assumed that the quantities in the physical model can be written as power series with respect to ε. Thereby, two different concepts are applied for different space directions:
In x_3-direction the existence of a fictive boundary layer is assumed, see Figure 5. For the velocity field v, the pressure p and the volume concentration $c^{\mathcal{V}}$ there are outer expansions , which are valid "far away" from the interface (far field), inner expansions for the boundary layer (near field) and matching conditions between them.
The inner expansions are coupled with periodic homogenization in the x_1-x_2-plane: It is assumed that the epitaxial layer forms an approximately periodic microstructure, see Figure 4. Therefore, asymptotic expansions for oscillations on the microscopic scale ε are assumed. This affects the elastic displacement field, the quantities of the BCF-model and the inner expansions of the fluid flow and the volumic transport process, but not their outer expansions. A microscopic space variable $y \in Y \times \mathbb{R}^+$ is introduced, where Y is a two dimensional periodicity cell, in the simplest case $Y = [(0,1)]^2$. The limit $y_3 \to \infty$ has to be

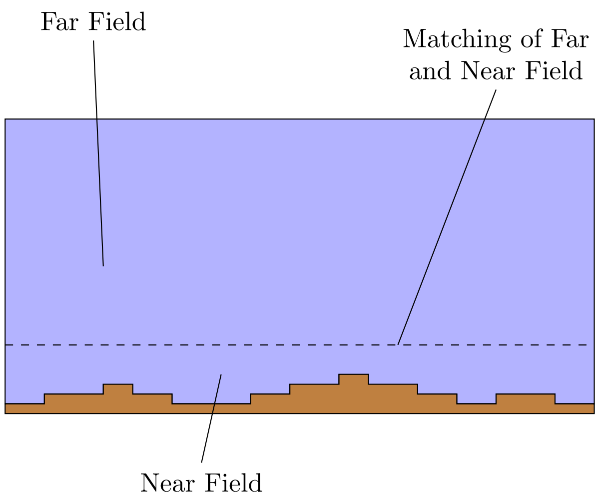


Figure 5: Inner and Outer Expansions.

interpreted as the "border" between near and far field. For the exact form of the expansions, the reader is referred to [10].
The "homogenized" domain for the macroscopic space variable x is Q, see Figure 6, and for any $x \in S_0$ there is a microscopic domain $Y \times \mathbb{R}^+$, which consists of the solid part

$$Q_l(x,t) = \{y \in \mathbb{R}^3 \mid (y_1, y_2) \in Y,\ y_3 > h_A \phi(t, x, y_1, y_2)\},$$

the liquid part

$$Q_s(x,t) = \{y \in \mathbb{R}^3 \mid (y_1, y_2) \in Y,\ 0 < y_3 < h_A \phi(t, x, y_1, y_2)\},$$

and the interface

$$\Gamma(x,t) = \{y \in \mathbb{R}^3 \mid (y_1, y_2) \in Y,\ y_3 = h_A \phi(t, x, y_1, y_2)\}.$$

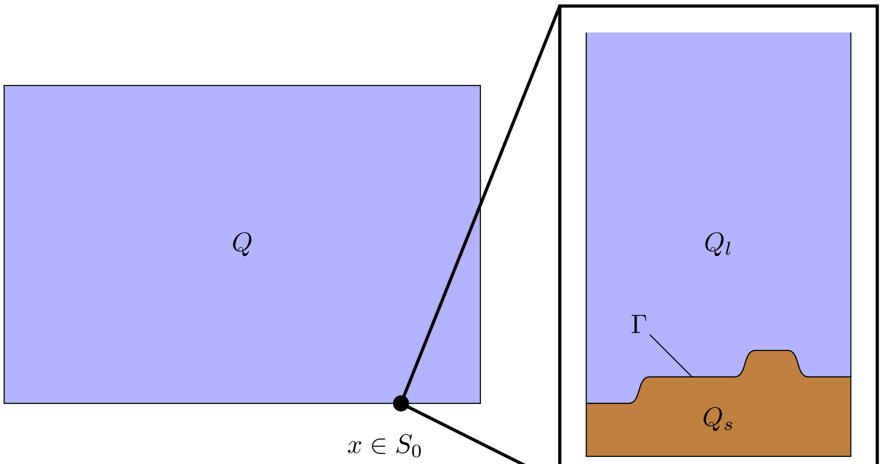


Figure 6: Macroscopic and Microscopic Domains.

Note, that $h_A \phi$ replaces the height function h for the description of the interface between solid layer and liquid solution. This is motivated by the interpretation of the phase field as the number of monomolecular layers over a point $y \in Y$, and by h_A as the height of one step.
The derivation of the two scale model works out as follows (see [10] for details): Insert the expansions into the model equations of section 2.1 and order by powers of ε. The unknowns in the model are

$v(x,t,y)$	:=	$v_1(x,t,y)$	microscopic fluid velocity
$V(x,t)$	:=	$V_0(t,x)$	macroscopic fluid velocity
$p(x,t,y)$	:=	$p_0(x,t,y)$	microscopic pressure
$P(x,t)$	:=	$P_0(x,t)$	macroscopic pressure
$C^{\mathcal{V}}(x,t)$	:=	$C_0^{\mathcal{V}}(x,t)$	volume concentration of particles in the liquid solution
$\phi(x,t,y)$	:=	$\phi_0(x,t,y)$	phase field
$c_s(x,t,y)$	:=	$c_{s,0}(x,t,y)$	surface concentration of adatoms
$u(x,t,y)$	:=	$u_0(x,t,y)$	elastic displacement

The index "0" denotes the term of lowest order of ε in the asymptotic expansions, the index "1" the next higher order. In order to simplify the notation, these indices are omitted from here on. Capital letters denote purely macroscopic quantities, small letters indicate quantities depending on x and y.
The model is composed of:

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

$$\begin{aligned} \operatorname{div}_x V = 0, \\ \partial_t V + (V \cdot \nabla_x)V - \eta \Delta_x V + \nabla_x P = 0, \end{aligned} \tag{2.21}$$

$$\partial_t C^{\mathcal{V}} + V \cdot \nabla_x C^{\mathcal{V}} - D^{\mathcal{V}} \Delta_x C^{\mathcal{V}} = 0. \tag{2.22}$$

Coupling conditions to the microscopic problems on $I \times S_0$ are

$$D^{\mathcal{V}} \frac{\partial C^{\mathcal{V}}}{\partial n} = \left(\frac{\bar{c}_s}{\tau_s} - \frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} \right), \tag{2.23}$$

$$V = 0, \tag{2.24}$$

where $\bar{c}_s(x,t) = \int_Y c_s(x,t,y)\,\mathrm{d}y$ is the microscopic mean value of c_s. Due to the boundary condition (2.24) the Navier-Stokes system (2.21) decouples from the other equations. Therefore, the velocity field V and the pressure P can be computed in a first step and then, the remaining problem has to be solved for given V and P. To complete the model, consider the boundary conditions

$$\frac{\partial C^{\mathcal{V}}}{\partial n} = 0, \tag{2.25}$$

$$V = 0, \tag{2.26}$$

on $I \times (\partial Q \setminus S_0)$, and initial conditions for $x \in Q$

$$C^{\mathcal{V}}(0,x) = C^{\mathcal{V}}_{ini}, \tag{2.27}$$

$$V(0,x) = V_{ini}. \tag{2.28}$$

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

$$\left. \begin{aligned} \operatorname{div}_y v = 0, \\ -\eta \Delta_y v + \nabla_y p = 0, \end{aligned} \right. \quad \text{in } Q_l, \tag{2.29}$$

with periodic boundary conditions for v with respect to y_1, y_2. Furthermore, there are two coupling conditions. On the free boundary Γ this is

$$v = v_\Gamma := -\left(\frac{1}{\varrho_{\mathcal{V}}} - \frac{1}{\varrho_E} \right) \left(\frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{c_s}{\tau_s} \right) e_3. \tag{2.30}$$

For $y_3 \to \infty$, there are the matching conditions

$$\lim_{y_3 \to \infty} \left(\nabla_y v + (\nabla_y v)^\top \right) e_3 = \left(\nabla_x V|_{x_3=0} + (\nabla_x V)^\top|_{x_3=0} \right) e_3, \tag{2.31}$$

$$\lim_{y_3 \to \infty} p = P|_{x_3=0}. \tag{2.32}$$

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

$$-\operatorname{div}_y \sigma_y(u) = 0, \quad \text{in } Q_s, \tag{2.33}$$

This system is completed by a Dirichlet boundary condition

$$u = b, \qquad \text{for} \quad y \in \tilde{\Gamma} := Y \times \{0\}, \tag{2.34}$$

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

$$\sigma_y(u)n - \eta\, e_y(v)\, n + pn = 0, \quad \text{on } \Gamma, \tag{2.35}$$

to the Stokes system. Here n is the outer normal vector on Q_s at Γ.

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

$$\tau\xi^2\partial_t\phi - \xi^2\Delta_y\phi + f'(\phi) + q(\phi, c_s, u) = 0, \tag{2.36}$$

$$\partial_t c_s + \varrho_s\partial_t\phi - D_s\Delta_y c_s = \frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{c_s}{\tau_s}, \tag{2.37}$$

with Y-periodic initial conditions

$$c_s(0, x, y) = c_{s,ini}(x, y), \qquad \phi(0, x, y) = \phi_{ini}(x, y), \tag{2.38}$$

and periodic boundary conditions with respect to y_1, y_2. The function f is the multi-well potential with minima at integer values, e.g. $f(\phi) = -\cos(2\pi\phi)$, and

$$q(\phi, c_s, u) = \frac{\xi R\mathcal{T}\varrho_s}{c_{\mathrm{eq}}\gamma\beta}(c_{\mathrm{eq}} - c_s)\, g_1'(\phi) + \frac{\xi h_A\varrho_s}{2c_{\mathrm{eq}}\gamma\beta}\sigma_y(u) : e_y(u), \tag{2.39}$$

where the function g_1' is either $g_1'(\phi) = \frac{1}{2}(1 - \cos(2\pi\phi))$ or $g_1'(\phi) = 1$. The first choice follows [15] and ensures that the corresponding term is only nonzero in the neighborhood of a step, while the second is that of [10].

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 S_0 one microscopic problem has to be solved. Since the microscopic problems at different macroscopic points do not influence each other directly, they can be solved in parallel computations. Furthermore, an adaptive strategy as in [24], where only few selected microscopic problems are solved, might be applicable: It requires continuous interscale dependencies, which are proven in sections 3. This reduces the computation effort significantly.

The above model is a first try to include elastic effects into the model of [6] and [8] without elasticity, and there is still room for discussion. It is not clear, for example, how to model the misfit between substrate and layer correctly. In [10], as in most foregone models, this is done as prescribed stress of the form

$$\sigma(u)n = b, \qquad \text{on } Y \times \{0\}, \tag{2.40}$$

while here, a prescribed displacement is assumed, see condition (2.34). The latter ensures uniqueness of the solution of the elasticity problem, while a solution for the Neumann condition (2.40) in combination with the Neumann condition (2.35) and periodic boundary conditions with respect to (y_1, y_2) can only be unique up to a constant. For the coupling to the rest of the model, this has no consequences, since only $e(u)$ appears there.

Furthermore, it is questionable, if any prescribed condition is correct at that point, or if rather an interaction between substrate and layer should be allowed, [27]. This would lead to another elasticity problem in the substrate with possibly another free boundary between substrate and layer.

Another point concerns the phase field and its coupling to the elastic part of the model. From the interpretation of ϕ, it is clear, that its values have to be nonnegative. But that can not be seen from the equation, especially due to the elastic term in (2.39). Furthermore, if the phase field is zero, the elastic energy term in (2.39) should vanish, since there is no solid layer left at that point. Moreover, the growth is modeled to take place at the steps. A possible approach here is to proceed as for the first term in (2.39) and to multiply the elastic term by a function $g_2'(\phi)$ which becomes zero for $\phi \in \mathbb{N}_0$, for example

$$g_2(\phi) = \frac{1}{2}\left(\phi - \frac{\sin(2\pi\phi)}{2\pi}\right),$$

compare g_1 in (2.15). The analysis of section 3 covers this choice, too.

3 Analysis

The well-posedness of the two scale model is investigated, existence and uniqueness of solutions are proven as main result. First, in 3.1, the solvability result is formulated in Theorem 3.1. A proof is presented in the subsequent sections 3.2, 3.3 and 3.4. It consists of two encapsulated fixed point arguments - an outer for the coupling between the microscopic and the macroscopic parts of the model and an inner for the coupled microscopic problem, see Figure 7.

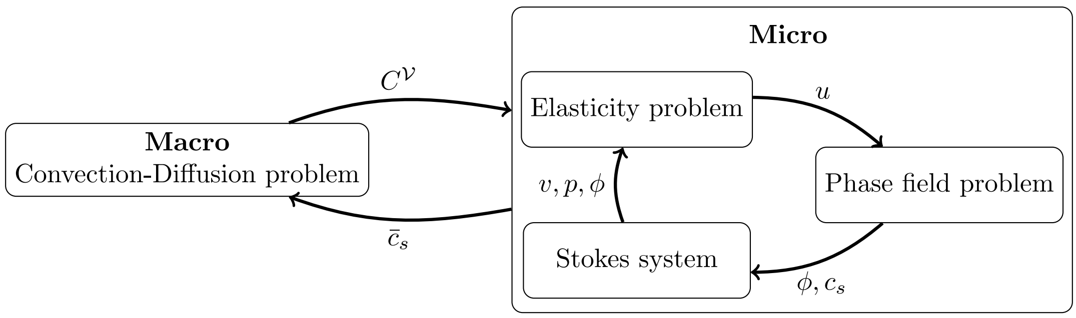


Figure 7: Strategy of the Proof of the Main Result: Encapsulated Fixed Point Iterations.

3.1 The Main Solvability Result

As already mentioned in section 2, the Navier-Stokes problem decouples from the rest of the model, due to condition (2.24). So, V and P can be precomputed before studying the other equations. The discussion of the solvability for the Navier-Stokes equations is not part of this article. In the textbooks [14, 29] an overview on solvability results for different boundary conditions can be found. In the following, V and P are considered as given, subject to suitable regularity assumptions as stated in the theorem.

Note furthermore, that the Stokes problem (2.29), (2.30), (2.31) and the elastic problem (2.33), (2.34), (2.35) 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* solutions (after proven to be existent) has to be investigated. This is not done on the time dependent domains $Q_l = Q_l(t)$ and $Q_s = Q_s(t)$, but on time independent domains $\hat{Q}_l$ and $\hat{Q}_s$. The corresponding (time dependent) domain transformations are denoted by

$$\Psi_l(t) \colon \hat{Q}_l \to Q_l(t), \qquad \Psi_s(t) \colon \hat{Q}_s \to Q_s(t). \tag{3.1}$$

The technical details are described in [11]. 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 $\hat{Q}_s$.

Furthermore in the following sections, many function spaces are provided with the lower index "per". This indicates functions which are periodic with respect to $(y_1, y_2) \in Y$, but there is no periodicity assumption on y_3.

The main theorem reads:

Theorem 3.1 (Existence and uniqueness of solutions of the fully coupled problem)**.** *Suppose* $V \in C^\beta(I, C(\overline{Q})) \cap C(I, C^1(\overline{Q}))$*,* $\beta > 0$*, and* $P \in C(I \times \overline{Q})$ *are solutions of the Navier-Stokes equations* (2.21), (2.24), (2.26) *and* (2.28)*. Assume furthermore that* $\phi_{ini}, c_{s,ini} \in C(S_0, C^{2+2\alpha}_{\text{per}}(Y))$*, with* $\phi_{ini}(y) > 0$ *for all* $y \in \overline{Y}$*,* $b \in C(I \times S_0, W^{2-1/r_1}_{r_1,\text{per}}(\tilde{\Gamma}))$ *and* $C^{\mathcal{V}}_{ini} \in W^1_{r_2}(Q)$*, where* $0 < \alpha < \frac{1}{2}$*,* $r_1 > \frac{6}{1-2\alpha}$ *and* $r_2 > 3$*,* $\frac{1}{r_2} + \frac{1}{r_2'} = 1$*. Then there exists locally in time, i.e. for a possibly reduced time interval* $I_{\tau_0} = [0, \tau_0]$*, a unique solution of the fully coupled two scale model* (2.22), (2.23), (2.25), (2.27) *and (2.29) – (2.38) in the following function spaces:*

$$\begin{aligned}
&\hat{v} \in C(I_{\tau_0} \times S_0, W^2_{r_1,\text{per},\text{loc}}(\hat{Q}_l)), && \phi \in C(S_0, C^{1,2+2\alpha}_{\text{per}}(I_{\tau_0} \times Y)),\\
&\hat{p} \in C(I_{\tau_0} \times S_0, W^1_{r_1,\text{per},\text{loc}}(\hat{Q}_l)), && c_s \in C(S_0, C^{1,2+2\alpha}_{\text{per}}(I_{\tau_0} \times Y)),\\
&\hat{u} \in C(I_{\tau_0} \times S_0, W^2_{r_1,\text{per}}(\hat{Q}_s)), && C^{\mathcal{V}} \in C^1\Big(I_{\tau_0}, (W^1_{r_2'}(Q))'\Big) \cap C\Big(I_{\tau_0}, W^1_{r_2}(Q)\Big).
\end{aligned}$$

The phase field ϕ *and the surface concentration* c_s *are classical solutions of their corresponding problems, while* v*,* p *and* u *are weak solutions. The volume concentration* $C^{\mathcal{V}}$ *is a bit of both: It is continuously differentiable in time, but the spatial differential operator is formulated in a weak sense.*

3.2 The Microscopic Problem

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 $C^{\mathcal{V}}(x, \cdot), V(x, \cdot), P(x, \cdot) \in C(I)$. These macroscopic quantities at a fixed point $x \in S_0$ are constant with respect to y.
First, sections 3.2.1–3.2.3 discuss the single parts of the microscopic problem: This is a review of the results in [11]. Section 3.2.4 studies the microscopic coupling with detailed proofs.
Concerning the notation: In some of the following estimates, the constant depends on the boundary of the corresponding domain and thus on ϕ (sometimes on two phase fields ϕ_1 and ϕ_2). It is stated explicitly in these cases. Mostly, this dependency will be expressed in terms of an upper bound $\kappa = \kappa(\phi)$ which satisfies

$$\kappa \geq \|\phi\|_{C(I,C^2(Y))} \qquad \text{or} \qquad \kappa \geq \max\{\|\phi_1\|_{C(I,C^2(Y))}, \|\phi_2\|_{C(I,C^2(Y))}\}, \tag{3.2}$$

depending on the context. In all estimates, where nothing like that is mentioned, the constants are independent of ϕ and of the other unknowns.

3.2.1 The Stokes Problem

Consider (2.29), (2.30) and (2.31). The existence and uniqueness of a weak solution is proven in [11] on the semi–infinite domain Q_l in suitable Hilbert spaces. In view of the coupling, further regularity studies are necessary, but only on a bounded subdomain $Q_{lK} \subset Q_l$, which is defined as

$$Q_{lK} := \{y \in Q_l \,|\, y_3 < h_A \phi(y_1, y_2) + K\}. \tag{3.3}$$

In fact, the behavior of v and p at infinity has no direct influence on the coupling to the elastic equation, only their regularity on Γ. Denote by (v, p) the unique weak solution of the Stokes problem (2.29), (2.30) and (2.31). Then, the following three statements can be proven analogously as in [11], section 5.1:

Theorem 3.2 (Spatial regularity)**.** *Consider fixed* $x \in S_0$ *and* $t \in I$*. Suppose* $2 \leq r < \infty$*,* $\phi(x,t) \in C^2_{\text{per}}(Y)$ *with* $\|\phi(x,t)\|_{C^2(Y)} \leq \kappa$*, with* κ *from* (3.2)*, and* $c_s(x,t) \in W^{2-1/r}_{r,\text{per}}(Y)$*. Then, the weak solution* $(v,p)(x,t)$ *of the Stokes problem satisfies* $v(x,t) \in \left[W^2_{r,\text{per}}(Q_{lK})\right]^3$*,* $p(x,t) \in W^1_{r,\text{per}}(Q_{lK})$*, and the a priori estimate*

$$\begin{aligned}
&\|v(x,t)\|_{W^2_r(Q_{lK})} + \|p(x,t)\|_{W^1_r(Q_{lK})}\\
&\leq c(\kappa)\left(\|c_s(x,t)\|_{W^{2-1/r}_r(Y)} + |C^{\mathcal{V}}(x,t)| + |\nabla V(x,t)| + |P(x,t)|\right).
\end{aligned} \tag{3.4}$$

In order to study the behavior of v and p with respect to time t, it is necessary to use the transformation Ψ_l from (3.1) and the transformed functions $\hat{v}$ and $\hat{p}$.

Theorem 3.3 (Regularity in space and time)**.** *Consider a fixed $x \in S_0$. Suppose $\phi(x) \in C(I, C^2_{\mathrm{per}}(Y))$ and $c_s(x) \in C(I, W^{2-1/r}_{r,\mathrm{per}}(Y))$. The solution (v, p) of the Stokes problem (2.29), (2.30), (2.31) satisfies*

$$\hat{v}(x) \in C(I, [W^2_{r,\mathrm{per}}(\hat{Q}_{lK})]^3), \qquad \hat{p}(x) \in C(I, W^1_{r,\mathrm{per}}(\hat{Q}_{lK})).$$

The estimate

$$\begin{aligned} &\|\hat{v}(x)\|_{C(I,W^2_r(\hat{Q}_{lK}))} + \|\hat{p}(x)\|_{C(I,W^1_r(\hat{Q}_{lK}))} \\ &\quad \le c(\kappa)\Big(\|c_s(x)\|_{C(I,W^{2-1/r}_r(Y))} + \|C^{\mathcal{V}}(x)\|_{C(I)} + \|\nabla_x V(x)\|_{C(I)} + \|P(x)\|_{C(I)}\Big) \end{aligned} \tag{3.5}$$

holds true, with κ from (3.2).

As last step, the dependency on the coupling data is investigated:

Lemma 3.4 (Continuity with respect to the coupling data)**.** *Suppose $c_{s,i}(x) \in C(I, W^{2-1/r}_{r,\mathrm{per}}(Y))$, $\phi_i(x) \in C(I, C^2_{\mathrm{per}}(Y))$ and $C^{\mathcal{V}}_i(x) \in C(I)$, $i = 1, 2$, and denote by $v_i(x), p_i(x)$ the corresponding solutions of the Stokes problem. Then, the estimate*

$$\begin{aligned} &\|(\hat{v}_1 - \hat{v}_2)(x)\|_{C(I,W^2_r(\hat{Q}_{lK}))} + \|(\hat{p}_1 - \hat{p}_2)(x)\|_{C(I,W^1_r(\hat{Q}_{lK}))} \\ &\quad \le c(\kappa)\Big(\|(\phi_1 - \phi_2)(x)\|_{C(I,C^2(Y))} + \|(c_{s,1} - c_{s,2})(x)\|_{C(I,W^{2-1/r}_r(Y))} + \|(C^{\mathcal{V}}_1 - C^{\mathcal{V}}_2)(x)\|_{C(I)}\Big) \end{aligned}$$

holds true, with κ from (3.2).

3.2.2 The Elasticity Problem

The discussion of the elasticity problem (2.33), (2.34), (2.35) is analogous to that of the Stokes problem. The proofs for the following results can either be found in [11], section 5.2, or easily adapted thereof. Existence and uniqueness of a weak solution, denoted by u, is proven in [11].

Theorem 3.5 (Spatial regularity)**.** *Consider fixed $x \in S_0$ and $t \in I$. Suppose that $\|\phi(x,t)\|_{C^2(Y)} < \kappa$ with $\phi(x,t,y) > 0$ for all $(x,t,y) \in S_0 \times I \times \overline{Y}$, $v(x,t) \in [W^2_{r,\mathrm{per}}(Q_{lK})]^3$, $p(x,t) \in W^1_{r,\mathrm{per}}(Q_{lK})$ and $b(x,t) \in [W^{2-1/r}_r(\tilde{\Gamma})]^3$ is the trace of a function $\bar{u}(x,t) \in [W^2_{r,\mathrm{per}}(Q_s)]^3$. Then, the weak solution $u(x,t)$ is an element of $[W^2_{r,\mathrm{per}}(Q_s)]^3$ and satisfies the a priori estimate*

$$\|u(x,t)\|_{W^2_r(Q_s)} \le c(\kappa)\left(\|v(x,t)\|_{W^2_r(Q_{lK})} + \|p(x,t)\|_{W^1_r(Q_{lK})} + \|b(x,t)\|_{W^{2-1/r}_r(\tilde{\Gamma})}\right). \tag{3.6}$$

Theorem 3.6 (Regularity in space and time)**.** *Consider a fixed $x \in S_0$. Suppose $\phi(x) \in C(I, C^2_{\mathrm{per}}(Y))$ with $\phi(x,t,y) > 0$ for all $(x,t,y) \in S_0 \times I \times \overline{Y}$, and $\hat{v}(x) \in C(I, [W^2_{r,\mathrm{per}}(\hat{Q}_{lK})]^3)$, $\hat{p}(x) \in C(I, W^1_{r,\mathrm{per}}(\hat{Q}_{lK}))$. The solution $u(x)$ of the elastic problem (2.33), (2.34), (2.35) satisfies*

$$\hat{u}(x) \in C(I, W^2_{r,\mathrm{per}}(\hat{Q}_s)),$$

and

$$\|\hat{u}(x)\|_{C(I,W^2_r(\hat{Q}_s))} \le c(\kappa)\Big(\|\hat{v}(x)\|_{C(I,W^2_r(\hat{Q}_{lK}))} + \|\hat{p}(x)\|_{C(I,W^1_r(\hat{Q}_{lK}))} + \|b(x)\|_{C(I,W^{2-1/r}_r(\tilde{\Gamma}))}\Big), \tag{3.7}$$

with κ from (3.2).

Lemma 3.7 (Continuity with respect to the coupling data)**.** *Suppose $\phi_i(x) \in C(I, C^2_{\mathrm{per}}(Y))$ with $\phi(x,t,y) > 0$ for all $(x,t,y) \in S_0 \times I \times \overline{Y}$, and $\hat{v}_i(x) \in C(I, [W^2_{r,\mathrm{per}}(\hat{Q}_{lK})]^3)$, $\hat{p}_i(x) \in C(I, W^1_{r,\mathrm{per}}(\hat{Q}_{lK}))$, $i = 1, 2$, and denote by $u_i(x)$ the corresponding solutions of the elastic problem. Then, the estimate*

$$\begin{aligned} \|(\hat{u}_1 - \hat{u}_2)(x)\|_{C(I,W^2_r(\hat{Q}_{lK}))} \le c(\kappa)\Big(&\|(\hat{v}_1 - \hat{v}_2)(x)\|_{C(I,W^2_r(\hat{Q}_{lK}))} + \|(\hat{p}_1 - \hat{p}_2)(x)\|_{C(I,W^1_r(\hat{Q}_{lK}))} \\ &+ \|(\phi_1 - \phi_2)(x)\|_{C(I,C^2(Y))}\Big), \end{aligned}$$

holds true, with κ from (3.2).

3.2.3 The Phase Field Problem

This section presents results on the solvability of the last part of the microscopic problem: the phase field version of the microscopic BCF-model (2.36) and (2.37) with initial conditions (2.38), and periodic boundary conditions with respect to $(y_1, y_2) \in Y$.
First, some remarks on the microscopic coupling data. There are two coupling quantities: The first is the elastic displacement field u which enters into the equations in (2.39). The second is κ from (3.2), which does not occur explicitly in the equations, but implicitly through u. Here, κ does not refer to the phase field, which is an unknown in this section, but to the phase field, that describes the boundary of the domain Q_s. The latter phase field is supposed to be given since u and Q_s are given.
Note furthermore, that the phase field problem is posed on a surface, and thus the coupling term $\sigma(u) : e(u)$ in (2.39) has to be understood in the trace sense. As explained in the beginning of section 3.1, the function $\hat{u} = u \circ \Psi_s$ is the transformed displacement field, defined on the time independent domain $\hat{Q}_s$ instead of the time dependent domain $Q_s(t)$. It is necessary to introduce $\hat{u}$ in order to define function spaces in time and space properly, as for example $C(I, [W^2_{r,\text{per}}(\hat{Q}_s)]^3)$. For the same reason, the coupling will be expressed in terms of $\hat{u}$ in what follows. Therefore write

$$\hat{q}(\phi, c_s, \hat{u}) := q(\phi, c_s, \hat{u} \circ \Psi_s^{-1}),$$

with q defined in (2.39).
The nonlinear terms f' and $\hat{q}$ in (2.36) satisfy the following growth and Lipschitz conditions, which can be easily verified:

$$|f'(\phi)| + |\hat{q}(\phi, c_s, \hat{u})| \leq c(\kappa) \left(1 + |\nabla \hat{u}|^2 + |c_s| + |\phi|\right), \tag{3.8}$$

$$\begin{aligned} |f'(\phi_1) - f'(\phi_2)| &+ |\hat{q}(\phi_1, c_{s,1}, \hat{u}_1) - \hat{q}(\phi_2, c_{s,2}, \hat{u}_2)| \\ &\leq c(\kappa) \left(|\phi_1 - \phi_2| + |c_{s,1} - c_{s,2}| + |\nabla(\hat{u}_1 + \hat{u}_2)|\, |\nabla(\hat{u}_1 - \hat{u}_2)|\right). \end{aligned} \tag{3.9}$$

The formulation of the coupling in terms of $\hat{u}$ instead of u causes the dependency of the constants in (3.8) and (3.9) on κ.
The following proofs only use the abstract conditions (3.8) and (3.9) and not the exact definitions of f and q. Thus, all of the following results hold for any functions f and q, which satisfy (3.8) and (3.9).
Consider test functions $w_1, w_2 \in L_2(I; H^1_{\text{per}}(Y))$, multiply equations (2.36) and (2.37) with w_1 and w_2 respectively, integrate by parts and get the following **weak formulation**:

Problem 3.8. *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 (2.38) are satisfied and for every $w_1, w_2 \in L_2(I; H^1_{\text{per}}(Y))$ the following equations hold true:*

$$\int_I \Big(\tau \xi^2 \langle \partial_t \phi, w_1 \rangle + \int_Y \left(\xi^2\, \nabla \phi \cdot \nabla w_1 + (f'(\phi) + \hat{q}(\phi, c_s, \hat{u}))\, w_1\right) \mathrm{d}y\Big) \mathrm{d}t = 0. \tag{3.10}$$

$$\int_I \left(\langle \partial_t c_s, w_2 \rangle + \varrho_s \langle \partial_t \phi, w_2 \rangle + \int_Y \left(D_s \nabla c_s \cdot \nabla w_2 + \left(\frac{c_s}{\tau_s} - \frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}}\right) w_2\right) \mathrm{d}y\right) \mathrm{d}t = 0, \tag{3.11}$$

Here, $\langle \cdot, \cdot \rangle$ denotes the dual pairing on $H^1_{\text{per}}(Y)$. There exists a unique solution with the following properties:

Theorem 3.9 (Existence and uniqueness of a weak solution of the phase field model)**.** *Assume $c_{s,ini}(x) \in L_2(Y)$, $\phi_{ini}(x) \in L_2(Y)$ and $\hat{u}(x) \in L_2(I, [W^2_{r,\text{per}}(\hat{Q}_s)]^3)$, for some $r \geq 3$. Furthermore, suppose that the constants D_s, τ, ξ, h_A, ϱ_s, $\tau^{\mathcal{V}}$ and τ_s are positive. Then, Problem 3.8 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 $(\phi, c_s)(x)$. It satisfies*

$$\begin{aligned} &\|\phi(x)\|_{L_\infty(I, L_2(Y))} + \|\phi(x)\|_{L_2(I, H^1(Y))} + \|c_s(x)\|_{L_\infty(I, L_2(Y))} + \|c_s(x)\|_{L_2(I, H^1(Y))} \\ &\quad \leq c(\kappa) \Big(1 + \|\hat{u}(x)\|^2_{L_2(I, W^2_r(\hat{Q}_s))} + \|C^{\mathcal{V}}(x)\|_{L_2(I)} + \|c_{s,ini}(x)\|_{L_2(Y)} + \|\phi_{ini}(x)\|_{L_2(Y)}\Big), \end{aligned} \tag{3.12}$$

with κ from (3.2).

Proof. The existence and uniqueness of a solution is proven in [11], Theorem 5.9. It remains to prove the a priori estimate (3.12).

Investigate first the regularity of the coupling term. Due to the growth condition (3.8), the crucial coupling term to study is $|\nabla\hat{u}|^2$, which has to be understood in the trace sense. Suppose $\hat{u} \in [W^2_{r,\mathrm{per}}(\hat{Q}_s)]^3$, for fixed t, then :

$$\hat{u} \in [W^2_r(\hat{Q}_s)]^3 \;\Rightarrow\; |\nabla\hat{u}|^2 \in W^1_{r/2}(\hat{Q}_s) \;\Rightarrow\; \mathrm{tr}\,|\nabla\hat{u}|^2 \in W^{1-2/r}_{r/2}(Y) \;\Rightarrow\; \mathrm{tr}\,|\nabla\hat{u}|^2 \in L_2(Y) \quad \text{if } r \geq 3.$$

For the norms there holds

$$\||\nabla\hat{u}|^2\|_{L_2(Y)} \leq c\||\nabla\hat{u}|^2\|_{W^{1-2/r}_{r/2}(Y)} \leq c\||\nabla\hat{u}|^2\|_{W^1_{r/2}(\hat{Q}_s)} \leq c\|\nabla\hat{u}\|^2_{W^1_r(\hat{Q}_s)} \leq c\|\hat{u}\|^2_{W^2_r(\hat{Q}_s)}, \tag{3.13}$$

which follows from the continuity of the trace operator $W^1_{r/2}(Q_s) \to W^{1-2/r}_{r/2}(Y)$ and the continuity of the embedding $W^{1-2/r}_{r/2}(Y) \hookrightarrow L_2(Y)$, with $r \geq 3$.

Set $w_1 = \chi_{I_{t_0}}\phi$ in (3.10) and use the growth condition (3.8) on f' and $\hat{q}$

$$|f'(\phi)| + |\hat{q}(\phi, c_s, \hat{u})| \leq c(\kappa)\left(1 + |\nabla\hat{u}|^2 + |c_s| + |\phi|\right).$$

Most of the following constants depend on κ, but for readability, this will be omitted in the notation for the moment. It follows

$$\begin{aligned}\|\phi(t_0)\|^2_{L_2(Y)} + \|\nabla\phi\|^2_{L_2(I_{t_0}\times Y)} \leq c\Big(&1 + \|\phi\|^2_{L_2(I_{t_0}\times Y)} + \|c_s\|^2_{L_2(I_{t_0}\times Y)} \\ &+ \||\nabla\hat{u}|^2\|^2_{L_2(I_{t_0}\times Y)} + \|\phi_{ini}\|^2_{L_2(Y)}\Big).\end{aligned} \tag{3.14}$$

Gronwall's inequality implies

$$\|\phi\|_{L_\infty(I_{t_0},L_2(Y))} \leq c\left(1 + \|c_s\|_{L_2(I_{t_0}\times Y)} + \||\nabla\hat{u}|^2\|_{L_2(I_{t_0}\times Y)} + \|\phi_{ini}\|_{L_2(Y)}\right). \tag{3.15}$$

Estimate (3.14) leads first to

$$\|\phi\|_{L_2(I_{t_0},H^1(Y))} \leq c\left(1 + \|\phi\|_{L_2(I_{t_0}\times Y)} + \|c_s\|_{L_2(I_{t_0}\times Y)} + \||\nabla\hat{u}|^2\|_{L_2(I_{t_0}\times Y)} + \|\phi_{ini}\|_{L_2(Y)}\right), \tag{3.16}$$

next with the continuous embedding $L_\infty(I_{t_0}, L_2(Y)) \hookrightarrow L_2(I_{t_0} \times Y)$ and (3.15) to

$$\|\phi\|_{L_2(I_{t_0},H^1(Y))} \leq c\left(1 + \|c_s\|_{L_2(I_{t_0}\times Y)} + \||\nabla\hat{u}|^2\|_{L_2(I_{t_0}\times Y)} + \|\phi_{ini}\|_{L_2(Y)}\right), \tag{3.17}$$

and finally with (3.10) to

$$\|\partial_t\phi\|_{L_2(I_{t_0},H^1(Y)')} \leq c\left(1 + \|c_s\|_{L_2(I_{t_0}\times Y)} + \||\nabla\hat{u}|^2\|_{L_2(I_{t_0}\times Y)} + \|\phi_{ini}\|_{L_2(Y)}\right). \tag{3.18}$$

Set now $w_2 = \chi_{I_{t_0}}c_s$ in (3.11) and use Young's inequality with $\varepsilon > 0$ to get

$$\begin{aligned}&\|c_s(t_0)\|^2_{L_2(Y)} + \|c_s\|^2_{L_2(I_{t_0},H^1(Y))} \\ &\leq c\Big(\|\partial_t\phi\|_{L_2(I_{t_0},H^1(Y)')}\|c_s\|_{L_2(I_{t_0},H^1(Y))} + \|c_s\|^2_{L_2(I_{t_0}\times Y)} + \|C^{\mathcal{V}}\|^2_{L_2(I_{t_0})} + \|c_{s,ini}\|^2_{L_2(Y)}\Big) \\ &\leq c\Big(c(\varepsilon)\|\partial_t\phi\|^2_{L_2(I_{t_0},H^1(Y)')} + \varepsilon\|c_s\|^2_{L_2(I_{t_0},H^1(Y))} + \|c_s\|^2_{L_2(I_{t_0}\times Y)} + \|C^{\mathcal{V}}\|^2_{L_2(I_{t_0})} + \|c_{s,ini}\|^2_{L_2(Y)}\Big).\end{aligned} \tag{3.19}$$

Choosing ε small enough allows to cancel the $\|c_s\|_{L_2(I_{t_0},H^1(Y))}$–term on the right-hand side of (3.19):

$$\|c_s(t_0)\|^2_{L_2(Y)} + \|c_s\|^2_{L_2(I_{t_0},H^1(Y))} \leq c\left(\|\partial_t\phi\|^2_{L_2(I_{t_0},H^1(Y)')} + \|c_s\|^2_{L_2(I_{t_0}\times Y)} + \|C^{\mathcal{V}}\|^2_{L_2(I_{t_0})} + \|c_{s,ini}\|^2_{L_2(Y)}\right).$$

Estimate (3.18) then yields

$$\|c_s(t_0)\|^2_{L_2(Y)} + \|c_s\|^2_{L_2(I_{t_0},H^1(Y))} \le c\Big(1 + \|c_s\|^2_{L_2(I_{t_0}\times Y)} + \||\nabla\hat{u}|^2\|^2_{L_2(I_{t_0}\times Y)} + \|C^{\mathcal{V}}\|^2_{L_2(I_{t_0})} + \|c_{s,ini}\|^2_{L_2(Y)} + \|\phi_{ini}\|^2_{L_2(Y)}\Big), \tag{3.20}$$

and thus with Gronwall's inequality

$$\|c_s\|_{L_\infty(I_{t_0},L_2(Y))} \le c\left(1 + \||\nabla\hat{u}|^2\|_{L_2(I_{t_0}\times Y)} + \|C^{\mathcal{V}}\|_{L_2(I_{t_0})} + \|c_{s,ini}\|_{L_2(Y)} + \|\phi_{ini}\|_{L_2(Y)}\right). \tag{3.21}$$

Combining (3.15), (3.17), (3.20) and (3.21) proves

$$\begin{aligned}\|\phi\|_{L_\infty(I_{t_0},L_2(Y))} + \|\phi\|_{L_2(I_{t_0},H^1(Y))} + \|c_s\|_{L_\infty(I_{t_0},L_2(Y))} + \|c_s\|_{L_2(I_{t_0},H^1(Y))}\\ \le c\Big(1+\|c_s\|_{L_2(I_{t_0}\times Y)} + \||\nabla\hat{u}|^2\|_{L_2(I_{t_0}\times Y)} + \|C^{\mathcal{V}}\|_{L_2(I_{t_0})} + \|c_{s,ini}\|_{L_2(Y)} + \|\phi_{ini}\|_{L_2(Y)}\Big).\end{aligned} \tag{3.22}$$

The embedding estimate

$$\|c_s\|_{L_2(I_{t_0}\times Y)} \le c\|c_s\|_{L_\infty(I_{t_0},L_2(Y))}$$

together with (3.13), (3.21) and (3.22) finally implies

$$\begin{aligned}\|\phi\|_{L_\infty(I_{t_0},L_2(Y))} + \|\phi\|_{L_2(I_{t_0},H^1(Y))} + \|c_s\|_{L_\infty(I_{t_0},L_2(Y))} + \|c_s\|_{L_2(I_{t_0},H^1(Y))}\\ \le c\left(1 + \|\hat{u}\|^2_{L_2(I_{t_0},W^2_r(\hat{Q}_s))} + \|C^{\mathcal{V}}\|_{L_2(I_{t_0})} + \|c_{s,ini}\|_{L_2(Y)} + \|\phi_{ini}\|_{L_2(Y)}\right),\end{aligned}$$

for any $0 < t_0 \le T$. Note, that c depends on κ from (3.8). □

Next, higher regularity is studied in the following Hölder spaces with anisotropic regularity in time and space: Suppose $0 < \alpha < \frac{1}{2}$, then

$$C^{1,2+2\alpha}(I\times Y) = \{f \in C(I\times Y)|\ \partial_t f, D^2 f \in C(I, C^{2\alpha}(Y))\}.$$

The first upper index always denotes the regularity in time, the second that in space.

Theorem 3.10 (Regularity)**.** *Suppose $0 < \alpha < \frac{1}{2}$, $r > \frac{6}{1-2\alpha}$ and $\phi_{ini}, c_{s,ini} \in C^{2+2\alpha}_{\mathrm{per}}(Y)$, and consider given $C^{\mathcal{V}} \in C(I)$ and u with $\hat{u} \in C(I, [W^2_{r,\mathrm{per}}(\hat{Q}_s)]^3)$. A solution (ϕ, c_s) of (2.36), (2.37), (2.38) belongs to $[C^{1,2+2\alpha}_{\mathrm{per}}(I\times Y)]^2$ with*

$$\|\phi(x)\|_{C^{1,2+2\alpha}(I\times Y)} + \|c_s(x)\|_{C^{1,2+2\alpha}(I\times Y)} \le c(\kappa)\Big(1 + \|C^{\mathcal{V}}(x)\|_{C(I)} + \|\hat{u}(x)\|^2_{C(I,W^2_r(\hat{Q}_s))} + \|\phi_{ini}(x)\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}(x)\|_{C^{2+2\alpha}(Y)}\Big), \tag{3.23}$$

with κ from (3.2)*.*

Proof. As in the proof of Theorem 3.9, start again with analogous considerations on the coupling term: Suppose $\hat{u} \in [W^2_{r,\mathrm{per}}(\hat{Q}_s)]^3$, for fixed t, then:

$$\begin{aligned}\hat{u} \in [W^2_r(Q_s)]^3 \quad &\Rightarrow \quad |\nabla\hat{u}|^2 \in W^1_{r/2}(Q_s)\\ &\Rightarrow \quad \mathrm{tr}\,|\nabla\hat{u}|^2 \in W^{1-2/r}_{r/2}(Y)\\ &\Rightarrow \quad \mathrm{tr}\,|\nabla\hat{u}|^2 \in C^{2\alpha}(Y), \quad \text{if } r > \tfrac{6}{1-2\alpha}, \text{ for some } 0 < \alpha < \tfrac{1}{2}.\end{aligned}$$

For the norms there holds

$$\||\nabla\hat{u}|^2\|_{C^{2\alpha}(Y)} \le c\||\nabla\hat{u}|^2\|_{W^{1-2/r}_{r/2}(Y)} \le c\||\nabla\hat{u}|^2\|_{W^1_{r/2}(\hat{Q}_s)} \le c\|\nabla\hat{u}\|^2_{W^1_r(\hat{Q}_s)} \le c\|\hat{u}\|^2_{W^2_r(\hat{Q}_s)}.$$

The key idea of the following proof is to use regularity results for the linear heat equation with homogeneous Dirichlet boundary conditions, namely Theorem 9.1 of Ch.IV in [17] and Theorem 5.1.13 in [20], and perform a bootstrap procedure:

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain such that $\overline{Y} \subset \Omega$ 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 $0 \leq \chi(y) \leq 1$ 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 (3.10) and (3.11) on $I \times Y$, then $\chi\phi$ and χc_s are weak solutions of

$$\tau\xi^2\partial_t(\chi\phi) - \xi^2\Delta(\chi\phi) = -\chi\left(f'(\phi) + \hat{q}(c_s, \hat{u}, \phi)\right) - \xi^2\left(\phi\Delta\chi + 2\nabla\chi\nabla\phi\right), \tag{3.24}$$

$$\partial_t(\chi c_s) - D_s\Delta(\chi c_s) = \chi\left(\frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{c_s}{\tau_s} - \varrho_s\partial_t\phi\right) - D_s\left(c_s\Delta\chi + 2\nabla\chi\nabla c_s\right) \tag{3.25}$$

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. The weak formulation of (3.24) and (3.25) is analogous to that in (3.10) and (3.11). From $c_s, \phi \in L_2(I, H^1(\Omega))$ it follows, that the righthand side of (3.24) is in $L_2(I\times\Omega)$, due to the growth condition (3.8) (This is also true if L_2 is replaced by any L_μ, $1 \leq \mu \leq \infty$). Omit again the dependency on κ in the following notation.
The application of Theorem 9.1 of Ch.IV in [17] yields

$$\chi\phi \in W_2^{1,2}(I \times \Omega),$$

with

$$\|\chi\phi\|_{W_2^{1,2}(I\times\Omega)} \leq c\Big(1 + \|\chi\phi\|_{L_2(I,H^1(\Omega))} + \|\chi c_s\|_{L_2(I\times\Omega)} + \|\chi|\nabla\hat{u}|^2\|_{L_2(I\times\Omega)} + \|\chi\phi_{ini}\|_{C^{2+2\alpha}(\Omega)}\Big).$$

From definition of χ and the Y–periodicity of the involved functions it follows $\phi \in W_2^{1,2}(I \times Y)$ with

$$\|\phi\|_{W_2^{1,2}(I\times Y)} \leq c\left(1 + \|\phi\|_{L_2(I,H^1(Y))} + \|c_s\|_{L_2(I\times Y)} + \|\hat{u}\|^2_{C(I,W_r^2(\hat{Q}_s))} + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)}\right). \tag{3.26}$$

The norms for $\hat{u}$ and ϕ_{ini} are not optimal at that point, but will be needed later. Note, that (3.26) implies $\partial_t\phi \in L_2(I \times Y)$, so the righthand side of (3.25) is in $L_2(I \times \Omega)$. Theorem 9.1 of Ch.IV in [17] can now be applied to equation (3.25) and this yields

$$c_s \in W_2^{1,2}(I \times Y),$$

with

$$\|c_s\|_{W_2^{1,2}(I\times Y)} \leq c\left(\|c_s\|_{L_2(I,H^1(Y))} + \|\partial_t\phi\|_{L_2(I\times Y)} + \|C^{\mathcal{V}}\|_{C(I)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)}\right). \tag{3.27}$$

For $0 < \lambda < 1$, there is the interpolatory inclusion

$$W_2^{1,2}(I \times Y) \hookrightarrow W_2^\lambda(I, W_2^{2(1-\lambda)}(Y))$$

with continuous embedding, see [7], Corollary 2.2.6. Furthermore, the embeddings

$$\begin{aligned} W_2^\lambda(I, W_2^{2(1-\lambda)}(Y)) &\hookrightarrow L_\mu(I, W_2^{2(1-\lambda)}(Y)), \quad \text{for} \quad && \lambda - \frac{1}{2} \geq -\frac{1}{\mu}, \\ W_2^{2(1-\lambda)}(Y) &\hookrightarrow W_\mu^1(Y), && \text{for} \quad 2(1-\lambda) - \frac{2}{2} \geq 1 - \frac{2}{\mu}, \end{aligned}$$

exist and are continuous, and therefore

$$W_2^{1,2}(I \times Y) \hookrightarrow W_2^\lambda(I, W_2^{2(1-\lambda)}(Y)) \hookrightarrow W_4^{0,1}(I \times Y)$$

with continuous embedding. It follows that $c_s, \phi \in W_4^{0,1}(I \times Y)$ with

$$\begin{aligned} \|\phi\|_{W_4^{0,1}(I\times Y)} + \|c_s\|_{W_4^{0,1}(I\times Y)} \leq c\Big(&1 + \|\phi\|_{L_2(I,H^1(Y))} + \|c_s\|_{L_2(I,H^1(Y))} + \|\hat{u}\|^2_{C(I,W_r^2(\hat{Q}_s))} \\ &+ \|C^{\mathcal{V}}\|_{C(I)} + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)}\Big). \end{aligned} \tag{3.28}$$

Repetition of the same argument for both equations in $L_4(I \times \Omega)$ instead of $L_2(I \times \Omega)$ implies $c_s, \phi \in W_4^{1,2}(I \times Y)$, and thus $c_s, \phi \in W_\mu^{0,1}(I \times Y)$, for all $1 \leq \mu < \infty$, due to the continuous embeddings $W_4^{1,2}(I \times Y) \hookrightarrow W_4^\lambda(I, W_4^{2(1-\lambda)}(Y)) \hookrightarrow W_\mu^{0,1}(I \times Y)$. Together with estimate (3.28) it follows

$$\begin{aligned}\|\phi\|_{W_\mu^{0,1}(I\times Y)} + \|c_s\|_{W_\mu^{0,1}(I\times Y)} \leq c\Big(&1 + \|\phi\|_{L_2(I,H^1(Y))} + \|c_s\|_{L_2(I,H^1(Y))} + \|\hat{u}\|^2_{C(I,W_r^2(\hat{Q}_s))} \\ &+ \|C^{\mathcal{V}}\|_{C(I)} + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)}\Big).\end{aligned} \tag{3.29}$$

Another application of Theorem 9.1 of Ch.IV in [17] yields $c_s, \phi \in W_\mu^{1,2}(I \times Y)$ for any $1 \leq \mu < \infty$, with

$$\begin{aligned}\|\phi\|_{W_\mu^{1,2}(I\times Y)} + \|c_s\|_{W_\mu^{1,2}(I\times Y)} \leq c\Big(&1 + \|\phi\|_{L_2(I,H^1(Y))} + \|c_s\|_{L_2(I,H^1(Y))} + \|\hat{u}\|^2_{C(I,W_r^2(\hat{Q}_s))} \\ &+ \|C^{\mathcal{V}}\|_{C(I)} + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)}\Big).\end{aligned} \tag{3.30}$$

Use again the interpolatory inclusion

$$W_\mu^{1,2}(I \times Y) \hookrightarrow W_\mu^\lambda(I, W_\mu^{2(1-\lambda)}(Y)), \qquad 0 < \lambda < 1, \tag{3.31}$$

with continuous embedding. The embeddings

$$\begin{aligned}W_\mu^\lambda(I, W_\mu^{2(1-\lambda)}(Y)) &\hookrightarrow C(I, W_\mu^{2(1-\lambda)}(Y)), \\ W_\mu^{2(1-\lambda)}(Y) &\hookrightarrow C^{1+2\alpha}(Y)\end{aligned}$$

exist and are continuous for $\lambda - \frac{1}{\mu} > 0$ and for $2(1-\lambda) - \frac{2}{\mu} > 1 + 2\alpha$. It follows that

$$W_\mu^\lambda(I, W_\mu^{2(1-\lambda)}(Y)) \hookrightarrow C(I, C^{1+2\alpha}(Y)), \tag{3.32}$$

for $\mu > \frac{4}{1-2\alpha}$, $0 < \alpha < \frac{1}{2}$, with continuous embedding. So the right-hand side of (3.24) belongs to $C^{0,2\alpha}(I \times \Omega)$ and vanishes on the boundary $\partial\Omega$, due to $\chi \in C_0^\infty(\Omega)$. Theorem 5.1.13 in [20] yields that $\chi\phi \in C^{1,2+2\alpha}(I \times \Omega)$ with

$$\begin{aligned}\|\chi\phi\|_{C^{1,2+2\alpha}(I\times\Omega)} \leq c\Big(&1+\|\chi\phi\|_{C^{0,1+2\alpha}(I\times\Omega)} + \|\chi c_s\|_{C^{0,2\alpha}(I\times\Omega)} \\ &+ \|\chi\hat{u}\|^2_{C(I,W_r^2(\hat{Q}_s))} + \|\chi\phi_{ini}\|_{C^{2+2\alpha}(\Omega)}\Big).\end{aligned} \tag{3.33}$$

Due to the just achieved regularity for ϕ, the right-hand side of (3.25) is also an element of $C^{0,2\alpha}(I \times \Omega)$ and vanishes on the boundary $\partial\Omega$. Consequently, combining Theorem 5.1.13 in [20] with (3.33), it is $\chi c_s \in C^{1,2+2\alpha}(I \times \Omega)$ with

$$\begin{aligned}\|\chi c_s\|_{C^{1,2+2\alpha}(I\times\Omega)} \leq c\Big(&1 + \|\chi\phi\|_{C^{0,1+2\alpha}(I\times\Omega)} + \|\chi c_s\|_{C^{0,1+2\alpha}(I\times\Omega)} + \|\chi\hat{u}\|^2_{C(I,W_r^2(\hat{Q}_s))} + \|C^{\mathcal{V}}\|_{C(I)} \\ &+ \|\chi\phi_{ini}\|_{C^{2+2\alpha}(\Omega)} + \|\chi c_{s,ini}\|_{C^{2+2\alpha}(\Omega)}\Big).\end{aligned} \tag{3.34}$$

The estimates (3.33) and (3.34), together with (3.12), (3.30), (3.31), (3.32) and the Y–periodicity of the involved functions imply, that

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

with

$$\begin{aligned}&\|\phi\|_{C^{1,2+2\alpha}(I\times Y)} + \|c_s\|_{C^{1,2+2\alpha}(I\times Y)} \\ &\quad \leq c\Big(1 + \|C^{\mathcal{V}}\|_{C(I)} + \|\hat{u}\|^2_{C(I,W_r^2(\hat{Q}_s))} + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)}\Big).\end{aligned} \tag{3.35}$$

The constant c depends on κ, since the constant in the growth condition (3.8) does, which was used in the proof. □

Lemma 3.11 (Continuity with respect to the coupling data)**.** *Suppose* $\hat{u}_1, \hat{u}_2 \in C(I, W^2_{r,\mathrm{per}}(\hat{Q}_s))$ *and* $C_1^{\mathcal{V}}, C_2^{\mathcal{V}} \in C(I)$*. Denote by* ϕ_1, ϕ_2 *and* $c_{s,1}, c_{s,2}$ *the corresponding solutions of* (2.36)- (2.38)*. The continuity estimate*

$$\begin{aligned} &\|(\phi_1 - \phi_2)(x)\|_{C^{1,2+2\alpha}(I\times Y)} + \|(c_{s,1} - c_{s,2})(x)\|_{C^{1,2+2\alpha}(I\times Y)} \\ &\quad \le c(\kappa)\Big(\|(\hat{u}_1 + \hat{u}_2)(x)\|_{C(I,W_r^2(\hat{Q}_s))}\|(\hat{u}_1 - \hat{u}_2)(x)\|_{C(I,W_r^2(\hat{Q}_s))} + \|(C_1^{\mathcal{V}} - C_2^{\mathcal{V}})(x)\|_{C(I)}\Big), \end{aligned} \tag{3.36}$$

holds true, with κ *from* (3.2)*.*

Proof. The proof for the continuity estimate (3.36) is analogous to that for the a priori estimates (3.12) and (3.23) with the following adaptions: If ϕ_1, ϕ_2 and $c_{s,1}, c_{s,2}$ solve (2.36)- (2.38) with corresponding $\hat{u}_1, \hat{u}_2$ and $C_1^{\mathcal{V}}, C_2^{\mathcal{V}}$, then $\tilde{\phi} := \phi_1 - \phi_2$ and $\tilde{c_s} := c_{s,1} - c_{s,2}$ solve

$$\begin{aligned} \tau\xi^2\partial_t\tilde{\phi} - \xi^2\Delta\tilde{\phi} + f'(\phi_1) - f'(\phi_2) + \hat{q}(c_{s,1}, \hat{u}_1, \phi_1) - \hat{q}(c_{s,2}, \hat{u}_2, \phi_2) = 0, \\ \partial_t\tilde{c}_s + \varrho_s\partial_t\tilde{\phi} - D_s\Delta\tilde{c}_s + \frac{\tilde{c}_s}{\tau_s} - \frac{C_1^{\mathcal{V}} - C_2^{\mathcal{V}}}{\tau^{\mathcal{V}}} = 0, \end{aligned}$$

with initial conditions $\tilde{c}_s(0, y) = \tilde{\phi}(0, y) = 0$, Proceeding as in the proofs for (3.12) and (3.23), using the Lipschitz condition (3.9) instead of the growth condition (3.8), finishes the proof. □

3.2.4 The Coupled Microscopic Problem

Throughout the following considerations, a point $x \in S_0$ is fixed and the macroscopic coupling data is supposed to be given, namely $C^{\mathcal{V}}(x, \cdot), \nabla V(x, \cdot), P(x, \cdot) \in C(I)$. The solvability of the elasticity equation is proven in section 3.2.2 under the assumption that $\phi(t, y) > 0$ for all $t \in I$ and $y \in \overline{Y}$. Thus define

$$M := \left\{\phi \in C(I, C^2_{\mathrm{per}}(Y)) \,\Big|\, \phi(t, y) > 0 \quad \forall t \in I,\ \forall y \in \overline{Y}\right\}.$$

Obviously, $\phi \in M$ implies $\phi(0, y) > 0$ for all $y \in \overline{Y}$. So the initial condition ϕ_{ini} needs to satisfy $\phi_{ini}(y) > 0$ for all $y \in \overline{Y}$. The results of the previous sections, namely Theorems 3.3, 3.6 and 3.10, allow the definition of the following solution operators:

$$\mathcal{S}_{\mathrm{Stokes}}\colon \begin{cases} M \times C(I, C^2_{\mathrm{per}}(Y)) & \to C(I, [W^2_{r,\mathrm{per}}(\hat{Q}_{lK})]^3 \times W^1_{r,\mathrm{per}}(\hat{Q}_{lK})) \times M \\ (\phi, c_s) & \mapsto (\hat{v}, \hat{p}, \phi), \end{cases}$$

$$\mathcal{S}_{\mathrm{elastic}}\colon \begin{cases} C(I, [W^2_{r,\mathrm{per}}(\hat{Q}_{lK})]^3 \times W^1_{r,\mathrm{per}}(\hat{Q}_{lK})) \times M & \to C(I, [W^2_{r,\mathrm{per}}(\hat{Q}_s)]^3) \\ (\hat{v}, \hat{p}, \phi) & \mapsto \hat{u}, \end{cases}$$

$$\mathcal{S}_{\mathrm{phasefield}}\colon \begin{cases} C(I, [W^2_{r,\mathrm{per}}(\hat{Q}_s)]^3) & \to [C^{1,2+2\alpha}_{\mathrm{per}}(I \times Y)]^2 \\ \hat{u} & \mapsto (\phi, c_s), \end{cases}$$

for some $0 < \alpha < \frac{1}{2}$ and $r > \frac{6}{1-2\alpha}$. The operator $\mathcal{S}_{\mathrm{Stokes}}$ maps ϕ onto itself (to define the composition $\mathcal{S}_{\mathrm{elastic}} \circ \mathcal{S}_{\mathrm{Stokes}}$). It will be proven that the composition

$$\mathcal{S} := \mathcal{S}_{\mathrm{phasefield}} \circ \mathcal{S}_{\mathrm{elastic}} \circ \mathcal{S}_{\mathrm{Stokes}}\colon \begin{cases} M \times C(I, C^2_{\mathrm{per}}(Y)) & \to [C^{1,2+2\alpha}_{\mathrm{per}}(I \times Y)]^2 \\ (\tilde{\phi}, \tilde{c_s}) & \mapsto (\phi, c_s) \end{cases}$$

has a unique fixed point. In order to apply Banach's fixed point theorem, it is necessary

i) to find a suitable nonempty and closed subset B of $M \times C(I, C^2_{\mathrm{per}}(Y))$, see Proposition 3.12, and

ii) to show that $\mathcal{S}$ maps B into itself, see Proposition 3.13, and

iii) to show that $\mathcal{S}\colon B \to B$ is a strict contraction, see Proposition 3.14.

The main tool in order to prove ii) and iii) is the reduction of the time interval, together with the a priori and continuity estimates for the single parts of the problem. The key in the proofs is the continuous embedding

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

see [20], Lemma 5.1.1, p.176, because it ensures that $\mathcal{S}(\phi, c_s) \in [C^{\alpha}(I, C^2(Y))]^2$ is more regular with respect to time than $(\phi, c_s) \in [C(I, C^2(Y))]^2$. The details are described hereafter.
Consider in the following a possibly reduced time interval $I_\tau = [0, \tau]$ with $0 < \tau \le T$ and set

$$M_{\tau,\alpha} := \left\{ \phi \in C^{\alpha}(I_\tau, C^2_{\text{per}}(Y)) \;\middle|\; \phi(t,y) > 0 \quad \forall t \in I_\tau,\ \forall y \in \overline{Y} \right\}.$$

Define

$$B_{R,\tau} = \Big\{ (\phi, c_s) \in \left[C^{\alpha}(I_\tau, C^2_{\text{per}}(Y))\right]^2 \;\Big|\; \|\phi\|_{C^{\alpha}(I_\tau, C^2(Y))} + \|c_s\|_{C^{\alpha}(I_\tau, C^2(Y))} \le R, \quad (\phi, c_s)(0, \cdot) = (\phi_{ini}, c_{s,ini}) \Big\},$$

for $R > \max\{\|\phi_{ini}\|_{C^2(Y)}, \|c_{s,ini}\|_{C^2(Y)}\}$. $B_{R,\tau}$ is a closed (with respect to the $C^{\alpha}(I_\tau, C^2(Y))$-norm) and nonempty set. Note, that $B_{R,\tau}$ is in general not a subset of $M_{\tau,\alpha} \times C^{\alpha}(I_\tau, C^2_{\text{per}}(Y))$, since $\phi(t,y) > 0$ is not necessarily fulfilled. $B_{R,\tau}$ complies with that only for certain choices of R and τ:

Proposition 3.12 (Well-definedness of $\mathcal{S}$ on $B_{R,\tau}$)**.** *Suppose $\phi_{ini}(y) > 0$ for all $y \in \overline{Y}$. For any $R > \max\{\|\phi_{ini}\|_{C^2(Y)}, \|c_{s,ini}\|_{C^2(Y)}\}$ there exists a time $\tau_1 > 0$, depending on R, such that*

$$B_{R,\tau_1} \subset M_{\tau_1,\alpha} \times C^{\alpha}(I_{\tau_1}, C^2_{\text{per}}(Y)).$$

Proof. It is to show that $(\phi, c_s) \in B_{R,\tau_1}$ implies $\phi(t,y) > 0$ for all $y \in \overline{Y}$ and $t \le \tau_1$, with a suitable $\tau_1 > 0$.
Consider an arbitrary but fixed $R > \max\{\|\phi_{ini}\|_{C^2(Y)}, \|c_{s,ini}\|_{C^2(Y)}\}$ and suppose $(\phi, c_s) \in B_{R,\tau}$. Then, ϕ is α–Hölder continuous in time with Hölder constant $\le R$. If $\phi_{ini}(y) > 0$ for all $y \in \overline{Y}$, then there exists $d := \min_{y \in \overline{Y}} \phi_{ini}(y) > 0$, because $\overline{Y}$ is compact. So,

$$|\phi(t,y) - \phi_{ini}(y)| \le R t^{\alpha},$$

and thus $\phi(t,y) > 0$ for all $y \in \overline{Y}$ and $t \le \tau_1 := \left(\frac{d}{2R}\right)^{1/\alpha}$. □

Proposition 3.12 ensures that the operator $\mathcal{S}\colon B_{R,\tau_1} \to [C^{1,2+2\alpha}_{\text{per}}(I \times Y)]^2$ is well-defined. Furthermore, there is a configuration of R and τ, such that $\mathcal{S}$ maps $B_{R,\tau}$ into itself:

Proposition 3.13 (Self-mapping)**.** *Suppose $\phi_{ini}(y) > 0$ for all $y \in \overline{Y}$. There exist postive numbers $R_0 > 0$ and $\tau_2 > 0$ such that*

$$\mathcal{S}\colon B_{R_0,\tau_2} \to B_{R_0,\tau_2}.$$

R_0 and τ_2 depend on the macroscopic coupling data, the initial data and the boundary data for the Stokes system and the elasticity equation.

Proof. Suppose $0 < \tau \le \tau_1$, with τ_1 from Proposition 3.12, and $(\tilde{\phi}, \tilde{c_s}) \in B_{R,\tau}$. Set $(\phi, c_s) = \mathcal{S}(\tilde{\phi}, \tilde{c_s})$. By construction of $\mathcal{S}$ it is $(\phi, c_s)(0, \cdot) = (\phi_{ini}, c_{s,ini})$.
It remains to show that $\|\phi\|_{C^{\alpha}(I_\tau, C^2(Y))} + \|c_s\|_{C^{\alpha}(I_\tau, C^2(Y))} \le R$: The a priori estimates for the single parts of the problem, see Theorems 3.3, 3.6 and 3.10, imply that

$$\begin{aligned} &\|\phi\|_{C^{1,2+2\alpha}(I_\tau \times Y)} + \|c_s\|_{C^{1,2+2\alpha}(I_\tau \times Y)} \\ &\qquad \le c(\kappa)\Big(1 + \|\tilde{c}_s\|^2_{C(I_\tau, C^2(Y))} + \|C^{\mathcal{V}}\|^2_{C(I_\tau)} + \|\nabla_x V\|^2_{C(I_\tau)} \\ &\qquad\quad + \|P\|^2_{C(I_\tau)} + \|b\|^2_{C(I_\tau, W_r^{2-1/r}(Y \times \{0\}))} + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)}\Big), \end{aligned} \tag{3.37}$$

where κ is an upper bound for $\|\tilde{\phi}\|_{C(I_\tau,C^2(Y))}$. For any $\tau \leq \tau_1$, κ can be choosen independently of $\tilde{\phi}$ and R: Due to $\tilde{\phi} \in C^\alpha(I_\tau, C^2_{\text{per}}(Y))$ and $\tau \leq \tau_1 = \left(\frac{d}{2R}\right)^{1/\alpha}$, with $d := \min_{y\in\overline{Y}} \phi_{ini}(y)$, it is for $0 \leq t \leq \tau$

$$\|\tilde{\phi}(t,y) - \phi_{ini}(y)\|_{C^2(Y)} \leq Rt^\alpha \leq \frac{d}{2}, \quad \text{and thus} \quad \sup_{t\in I_\tau} \|\tilde{\phi}(t)\|_{C^2(Y)} \leq \|\phi_{ini}\|_{C^2(Y)} + \frac{d}{2} =: \kappa.$$

So, the constant c in (3.37) can be choosen independently of $\tilde{\phi}$ and R, and (3.37) can be written as

$$\|\phi\|_{C^{1,2+2\alpha}(I_\tau\times Y)} + \|c_s\|_{C^{1,2+2\alpha}(I_\tau\times Y)} \leq c_1(C^{\mathcal{V}}, V, P, b, \phi_{ini}, c_{s,ini}) + c_2\|\tilde{c}_s\|^2_{C(I_\tau,C^2(Y))}, \tag{3.38}$$

where

$$c_1(C^{\mathcal{V}}, V, P, b, \phi_{ini}, c_{s,ini}) = c\Big(1 + \|C^{\mathcal{V}}\|^2_{C(I)} + \|\nabla_x V\|^2_{C(I)} + \|P\|^2_{C(I)} + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)} + \|b\|^2_{C(I,W_r^{2-1/r}(Y\times\{0\}))}\Big).$$

Next, note that

$$\|\tilde{c_s}\|_{C(I_\tau,C^2(Y))} = \max_{t\in I_\tau} \|\tilde{c_s}(t) - c_{s,ini} + c_{s,ini}\|_{C^2(Y)} \leq R\tau^\alpha + \|c_{s,ini}\|_{C^2(Y)}.$$

Consequently, (3.38) becomes

$$\|\phi\|_{C^{1,2+2\alpha}(I_\tau\times Y)} + \|c_s\|_{C^{1,2+2\alpha}(I_\tau\times Y)} \leq \tilde{c}_1(C^{\mathcal{V}}, V, P, b, \phi_{ini}, c_{s,ini}) + \tilde{c}_2 R^2\tau^{2\alpha}, \tag{3.39}$$

with

$$\tilde{c}_1(C^{\mathcal{V}}, V, P, b, \phi_{ini}, c_{s,ini}) = c_1(C^{\mathcal{V}}, V, P, b, \phi_{ini}, c_{s,ini}) + \tilde{c}_2\|c_{s,ini}\|^2_{C^2(Y)}.$$

The continuous embedding $C^{1,2+2\alpha}(I_\tau \times Y) \hookrightarrow C^\alpha(I_\tau, C^2(Y))$, see [20], Lemma 5.1.1, p.176, implies together with (3.39) that

$$\begin{aligned}\|\phi\|_{C^\alpha(I_\tau,C^2(Y))} + \|c_s\|_{C^\alpha(I_\tau,C^2(Y))} &\leq c_3\left(\|\phi\|_{C^{1,2+2\alpha}(I_\tau\times Y)} + \|c_s\|_{C^{1,2+2\alpha}(I_\tau\times Y)}\right) \\ &\leq c_3\tilde{c}_1(C^{\mathcal{V}}, V, P, b, \phi_{ini}, c_{s,ini}) + c_3\tilde{c}_2 R^2\tau^{2\alpha}.\end{aligned} \tag{3.40}$$

Choose now $R_0 := 2\tilde{c}_1 c_3$ and $\tau_2 > 0$ such that $\tilde{c}_2 c_3 R_0 \tau_2^{2\alpha} \leq \frac{1}{2}$, i.e. $\tau_2 \leq (2\tilde{c}_2 c_3 R_0)^{-\frac{1}{2\alpha}}$. It follows from (3.40) that

$$\|\phi\|_{C^\alpha(I_{\tau_2},C^2(Y))} + \|c_s\|_{C^\alpha(I_{\tau_2},C^2(Y))} \leq R_0.$$

□

Finally, there is a choice of R and τ such that $\mathcal{S}\colon B_{R,\tau} \to B_{R,\tau}$ is a strict contraction:

Proposition 3.14 (Contraction)**.** *Consider R_0 from Proposition 3.13. There exists a number $\tau_3 > 0$ such that the operator*

$$\mathcal{S}\colon B_{R_0,\tau_3} \to B_{R_0,\tau_3}$$

is a strict contraction.

Proof. Suppose $0 < \tau \leq \tau_2$, with τ_2 from Proposition 3.13, and $(\tilde{\phi}_i, \tilde{c}_{s,i}) \in B_{R_0,\tau}$, $i = 1, 2$. Set $(\phi_i, c_{s,i}) = \mathcal{S}(\tilde{\phi}_i, \tilde{c}_{s,i})$. The continuity estimates of Lemmata 3.4, 3.7 and 3.11 (with $C_1^{\mathcal{V}} = C_2^{\mathcal{V}}$) imply that

$$\begin{aligned}&\|\phi_1 - \phi_2\|_{C^{1,2+2\alpha}(I_\tau\times Y)} + \|c_{s,1} - c_{s,2}\|_{C^{1,2+2\alpha}(I_\tau\times Y)} \\ &\quad\leq c(\kappa)\|\hat{u}_1 + \hat{u}_2\|_{C(I,W_r^2(\hat{Q}_s))}\left(\|\tilde{\phi}_1 - \tilde{\phi}_2\|_{C(I_\tau,C^2(Y))} + \|\tilde{c}_{s,1} - \tilde{c}_{s,2}\|_{C(I_\tau,C^2(Y))}\right),\end{aligned}$$

where $\hat{u}_i = \mathcal{S}_{elastic} \circ \mathcal{S}_{Stokes}(\tilde{\phi}_i, \tilde{c}_{s,i})$ and $\kappa \geq \max\{\|\tilde{\phi}_1\|_{C(I_\tau,C^2(Y))}, \|\tilde{\phi}_2\|_{C(I_\tau,C^2(Y))}\}$. As seen in the proof of Proposition 3.13, κ can be choosen independently of $\tilde{\phi}_i \in B_{R_0,\tau}$, if $\tau \leq \tau_1$, with τ_1 from Proposition

3.12. This is satisfied here. Furthermore, the a priori estimates of Theorems 3.3 and 3.6 yield together with $(\tilde{\phi}_i, \tilde{c}_{s,i}) \in B_{R_0,\tau}$

$$\begin{aligned}\|\hat{u}_1 + \hat{u}_2\|_{C(I_\tau, W_r^2(\hat{Q}_s))} \leq & c_1(\kappa, C^{\mathcal{V}}, \nabla V, P, b) + c_2(\kappa)\left(\|\tilde{c}_{s,1}\|_{C(I_\tau, C^2(Y))} + \|\tilde{c}_{s,2}\|_{C(I_\tau, C^2(Y))}\right) \\ \leq & c_1(\kappa, C^{\mathcal{V}}, \nabla V, P, b) + 2c_2(\kappa)R_0 \\ \leq & c(\phi_{ini}, c_{s,ini}, C^{\mathcal{V}}, \nabla V, P, b, R_0).\end{aligned}$$

This leads to

$$\begin{aligned}&\|\phi_1 - \phi_2\|_{C^{1,2+2\alpha}(I_\tau \times Y)} + \|c_{s,1} - c_{s,2}\|_{C^{1,2+2\alpha}(I_\tau \times Y)} \\ &\qquad \leq c\left(\|\tilde{\phi}_1 - \tilde{\phi}_2\|_{C(I_\tau, C^2(Y))} + \|\tilde{c}_{s,1} - \tilde{c}_{s,2}\|_{C(I_\tau, C^2(Y))}\right),\end{aligned}$$

with a constant c only depending on initial, boundary and macroscopic coupling data. By construction, it is $(\tilde{\phi}_1 - \tilde{\phi}_2)(0, y) = (\tilde{c}_{s,1} - \tilde{c}_{s,2})(0, y) = 0$, and since $\tilde{\phi}_i$ and $\tilde{c}_{s,i}$ belong to $C^\alpha(I_\tau, C^2(Y))$, it follows

$$\begin{aligned}\|\tilde{\phi}_1 - \tilde{\phi}_2\|_{C(I_\tau, C^2(Y))} &\leq \tau^\alpha \|\tilde{\phi}_1 - \tilde{\phi}_2\|_{C^\alpha(I_\tau, C^2(Y))}, \\ \|\tilde{c}_{s,1} - \tilde{c}_{s,2}\|_{C(I_\tau, C^2(Y))} &\leq \tau^\alpha \|\tilde{c}_{s,1} - \tilde{c}_{s,2}\|_{C^\alpha(I_\tau, C^2(Y))},\end{aligned}$$

and consequently

$$\begin{aligned}&\|\phi_1 - \phi_2\|_{C^{1,2+2\alpha}(I_\tau \times Y)} + \|c_{s,1} - c_{s,2}\|_{C^{1,2+2\alpha}(I_\tau \times Y)} \\ &\qquad \leq c\tau^\alpha \left(\|\tilde{\phi}_1 - \tilde{\phi}_2\|_{C^\alpha(I_\tau, C^2(Y))} + \|\tilde{c}_{s,1} - \tilde{c}_{s,2}\|_{C^\alpha(I_\tau, C^2(Y))}\right).\end{aligned}$$

The continuous embedding $C^{1,2+2\alpha}(I_\tau \times Y) \hookrightarrow C^\alpha(I_\tau, C^2(Y))$, see [20], Lemma 5.1.1, p.176, implies

$$\begin{aligned}&\|\phi_1 - \phi_2\|_{C^\alpha(I_\tau, C^2(Y))} + \|c_{s,1} - c_{s,2}\|_{C^\alpha(I_\tau, C^2(Y))} \\ &\qquad \leq \tilde{c}\tau^\alpha \left(\|\tilde{\phi}_1 - \tilde{\phi}_2\|_{C^\alpha(I_\tau, C^2(Y))} + \|\tilde{c}_{s,1} - \tilde{c}_{s,2}\|_{C^\alpha(I_\tau, C^2(Y))}\right).\end{aligned}$$

Choose now τ_3 such that $\tilde{c}\tau_3^\alpha < 1$. This finishes the proof. □

Now, everything is prepared to prove the solvability of the coupled microscopic problem as the most important result in section 3.2:

Theorem 3.15 (Existence and uniqueness of a solution of the coupled microscopic problem)**.** *Suppose $C^{\mathcal{V}}(x, \cdot), \nabla_x V(x, \cdot), P(x, \cdot) \in C(I_{\tau_3})$ for $x \in S_0$, with τ_3 from Proposition 3.14. Assume furthermore that*

$$b(x, \cdot, \cdot) \in C(I_{\tau_3}, W_{r,\mathrm{per}}^{2-1/r}(Y \times \{0\})), \quad \phi_{ini}(x, \cdot), c_{s,ini}(x, \cdot) \in C_{\mathrm{per}}^{2+2\alpha}(Y),$$

with $\phi_{ini}(x, y) > 0$ for all $y \in \overline{Y}$. Then, there exists a unique solution $(\phi, c_s, v, p, u)(x)$ of (2.29) – (2.38) with

$$\begin{aligned}&\phi(x), c_s(x) \in C_{\mathrm{per}}^{1,2+2\alpha}(I_{\tau_3} \times Y), && \hat{u}(x) \in C(I_{\tau_3}, [W_{r,\mathrm{per}}^2(\hat{Q}_s)]^3), \\ &\hat{v}(x) \in C(I_{\tau_3}, [W_{r,\mathrm{per}}^2(\hat{Q}_{lK})]^3), && \hat{p}(x) \in C(I_{\tau_3}, W_{r,\mathrm{per}}^1(\hat{Q}_{lK})),\end{aligned}$$

for some $0 < \alpha < \frac{1}{2}$, $r > \frac{6}{1-2\alpha}$. This solution satisfies the a priori estimate

$$\begin{aligned}&\|\phi(x)\|_{C^{1,2+2\alpha}(I_{\tau_3} \times Y)} + \|c_s(x)\|_{C^{1,2+2\alpha}(I_{\tau_3} \times Y)} + \|\hat{v}(x)\|_{C(I_{\tau_3}, W_{r,\mathrm{per}}^2(\hat{Q}_{lK}))} \\ &\quad + \|\hat{p}(x)\|_{C(I_{\tau_3}, W_{r,\mathrm{per}}^1(\hat{Q}_{lK}))} + \|\hat{u}(x)\|_{C(I_{\tau_3}, W_{r,\mathrm{per}}^2(\hat{Q}_s))} \\ &\quad \leq c\Big(1 + \|C^{\mathcal{V}}(x)\|_{C(I_{\tau_3})}^2 + \|\nabla_x V(x)\|_{C(I_{\tau_3})}^2 + \|P(x)\|_{C(I_{\tau_3})}^2 \\ &\qquad + \|b(x)\|_{C(I_{\tau_3}, W_r^{2-1/r}(Y \times \{0\}))}^2 + \|\phi_{ini}(x)\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}(x)\|_{C^{2+2\alpha}(Y)}^2\Big).\end{aligned} \tag{3.41}$$

Proof. The assumptions for Banach's fixed point theorem on the operator $\mathcal{S}\colon B_{R_0,\tau_3} \to B_{R_0,\tau_3}$ are fulfilled and so, there exists a unique fixed point in B_{R_0,τ_3}. Any fixed point (ϕ, c_s) of $\mathcal{S}$, together with $(\hat{v},\hat{p}) = \mathcal{S}_{\text{Stokes}}(\phi, c_s)$ and $\hat{u} = \mathcal{S}_{\text{elastic}}(\hat{v},\hat{p},\phi)$ solves (2.29) – (2.38). Due to Theorems 3.3, 3.6 and 3.10, it is

$$\phi(x), c_s(x) \in C^{1,2+2\alpha}_{\text{per}}(I_{\tau_3} \times Y).$$

As seen in Proposition 3.13, (ϕ, c_s) satisfy

$$\|\phi\|_{C^{1,2+2\alpha}(I_{\tau_3}\times Y)} + \|c_s\|_{C^{1,2+2\alpha}(I_{\tau_3}\times Y)} \le cR_0.$$

By the definition of R_0 in the proof of Proposition 3.13 and the estimates of Lemmata 3.3, 3.6 it follows (3.41).
It remains to show that the found solution is unique not only in B_{R_0,τ_3}, but also in $M \times C(I_{\tau_3}, C^2_{\text{per}}(Y))$. Suppose therefore that $(\phi_i, c_{s,i}) \in M \times C(I_{\tau_3}, C^2_{\text{per}}(Y))$, $i = 1, 2$, are fixed points of $\mathcal{S}$. Note, that $(\phi_i, c_{s,i})$ also belong to $C^{1,2+2\alpha}_{\text{per}}(I_{\tau_3} \times Y)$, due to Theorems 3.3, 3.6 and 3.10, and thus to $C^\alpha(I_{\tau_3}, C^2_{\text{per}}(Y))$. Since $(\phi_i, c_{s,i})$ satisfy the same initial condition, it is $\|(\phi_1 - \phi_2)(0)\|_{C^2(Y)} = 0$ and $\|(c_{s,1} - c_{s,2})(0)\|_{C^2(Y)} = 0$. As seen in Proposition 3.14, the estimate

$$\begin{aligned}&\|\phi_1 - \phi_2\|_{C^\alpha(I_\tau,C^2(Y))} + \|c_{s,1} - c_{s,2}\|_{C^\alpha(I_\tau,C^2(Y))}\\ &\le c(\kappa)\tau^\alpha \|\hat{u}_1 + \hat{u}_2\|_{C(I_\tau,W^2_r(\hat{Q}_s))} \left(\|\phi_1 - \phi_2\|_{C^\alpha(I_\tau,C^2(Y))} + \|c_{s,1} - c_{s,2}\|_{C^\alpha(I_\tau,C^2(Y))}\right),\end{aligned}$$

is satisfied for any $\tau \in I_{\tau_3}$, where $\kappa \ge \max\{\|\phi_1\|_{C(I_{\tau_3},C^2(Y))}, \|\phi_2\|_{C(I_{\tau_3},C^2(Y))}\}$. It follows that $\|(\phi_1 - \phi_2)(t)\|_{C^2(Y)} = \|(c_{s,1} - c_{s,2})(t)\|_{C^2(Y)} = 0$ for $t \in [0, \tau]$, if

$$c(\kappa)\tau^\alpha \|\hat{u}_1 + \hat{u}_2\|_{C(I_\tau,W^2_r(\hat{Q}_s))} < 1.$$

Repeat the argument to show that $\|(\phi_1 - \phi_2)(t)\|_{C^2(Y)} = \|(c_{s,1} - c_{s,2})(t)\|_{C^2(Y)} = 0$ not only on $[0, \tau]$: If $\|(\phi_1 - \phi_2)(t_0)\|_{C^2(Y)} = \|(c_{s,1} - c_{s,2})(t_0)\|_{C^2(Y)} = 0$ for some $t_0 \in I_{\tau_3}$ then it is $\|(\phi_1 - \phi_2)(t)\|_{C^2(Y)} = \|(c_{s,1} - c_{s,2})(t)\|_{C^2(Y)} = 0$ for all $t \in [t_0, t_0 + \tau(t_0)] \cap I_{\tau_3}$. This shows that the set

$$I' := \left\{t \in I_{\tau_3} \,\middle|\, \|(\phi_1 - \phi_2)(t)\|_{C^2(Y)} = \|(c_{s,1} - c_{s,2})(t)\|_{C^2(Y)} = 0\right\}$$

is an open subset of I_{τ_3}. It is not empty because $0 \in I'$. But since $t \mapsto \|(\phi, c_s)(t)\|_{C^2(Y)}$ is continuous, I' is also closed in I_{τ_3} and therefore $I' = I_{\tau_3}$. This proves uniqueness of the solution of (2.29) – (2.38). ☐

With the statement of Theorem 3.15, the main goal concerning the analysis for the microscopic problem is reached, while a macroscopic point $x \in S_0$ was fixed. This section ends with necessary preparations for the micro-macro-coupling: Investigation of the regularity with respect to $x \in S_0$ and continuity with respect to the coupling data. The answers are formulated in the following Lemmata:

Lemma 3.16 (Regularity with respect to $x \in S_0$)**.** *Suppose that $C^{\mathcal{V}}$, $\nabla_x V$, P, b, ϕ_{ini} and $c_{s,ini}$ depend continuously on $x \in S_0$. Then, the solution of (2.29) – (2.38) depends continuously on $x \in S_0$ and*

$$\begin{aligned}&\|\phi\|_{C(S_0,C^{1,2+2\alpha}(I_{\tau_3}\times Y))} + \|c_s\|_{C(S_0,C^{1,2+2\alpha}(I_{\tau_3}\times Y))} + \|\hat{v}\|_{C(I_{\tau_3}\times S_0,W^2_{r,\text{per}}(\hat{Q}_{lK}))}\\ &\qquad + \|\hat{p}\|_{C(I_{\tau_3}\times S_0,W^1_{r,\text{per}}(\hat{Q}_{lK}))} + \|\hat{u}\|_{C(I_{\tau_3}\times S_0,W^2_{r,\text{per}}(\hat{Q}_s))}\\ &\quad\le c\Big(1 + \|C^{\mathcal{V}}\|^2_{C(I_{\tau_3}\times S_0)} + \|b\|^2_{C(I_{\tau_3}\times S_0,W^{2-1/r}_r(Y\times\{0\}))} + \|\nabla_x V\|^2_{C(I_{\tau_3}\times S_0)}\\ &\qquad + \|P\|^2_{C(I_{\tau_3}\times S_0)} + \|\phi_{ini}\|_{C(S_0,C^{2+2\alpha}(Y))} + \|c_{s,ini}\|^2_{C(S_0,C^{2+2\alpha}(Y))}\Big).\end{aligned} \tag{3.42}$$

Proof. Suppose for $i = 1, 2$ points $x_i \in S_0$ and set $C^{\mathcal{V}}_i = C^{\mathcal{V}}(x_i)$, $\phi_i = \phi(x_i)$ and $c_{s,i} = c_s(x_i)$. Analogously to the proof of Proposition 3.14 it holds for $\tau \in I_{\tau_3}$

$$\begin{aligned}&\|\phi_1 - \phi_2\|_{C^\alpha(I_\tau,C^2(Y))} + \|c_{s,1} - c_{s,2}\|_{C^\alpha(I_\tau,C^2(Y))}\\ &\le c\left(\tau^\alpha \left(\|\phi_1 - \phi_2\|_{C^\alpha(I_\tau,C^2(Y))} + \|c_{s,1} - c_{s,2}\|_{C^\alpha(I_\tau,C^2(Y))}\right) + \|C^{\mathcal{V}}_1 - C^{\mathcal{V}}_2\|_{C(I_\tau)}\right),\end{aligned} \tag{3.43}$$

with a constant $c > 0$ depending only on the initial, boundary and macroscopic coupling data. As long as $c\tau^\alpha < 1$, it follows

$$\|\phi_1 - \phi_2\|_{C^\alpha(I_\tau, C^2(Y))} + \|c_{s,1} - c_{s,2}\|_{C^\alpha(I_\tau, C^2(Y))} \le c\|C_1^{\mathcal{V}} - C_2^{\mathcal{V}}\|_{C(I_\tau)}.$$

Repeating these arguments, starting with arbitrary $t_0 \in I_{\tau_3}$ as initial time, leads to an analogous estimate as (3.43) on the time interval $[t_0, t_0 + \tau] \cap I_{\tau_3}$, with a constant $\tilde{c}$ depending on $\|\phi_i(t_0)\|_{C^{2+2\alpha}(Y)}$ and $\|c_{s,i}(t_0)\|_{C^{2+2\alpha}(Y)}$ instead of $\|\phi_i(0)\|_{C^{2+2\alpha}(Y)}$ and $\|c_{s,i}(0)\|_{C^{2+2\alpha}(Y)}$. Thanks to the a priori estimate (3.41), the mentioned constant $\tilde{c}$ can in fact be choosen independently of t_0, such that

$$\|\phi_1 - \phi_2\|_{C^\alpha([t_0,t_0+\tau], C^2(Y))} + \|c_{s,1} - c_{s,2}\|_{C^\alpha([t_0,t_0+\tau], C^2(Y))} \le c\|C_1^{\mathcal{V}} - C_2^{\mathcal{V}}\|_{C([t_0,t_0+\tau])},$$

as long as $t_0 + \tau \le \tau_3$ and $\tilde{c}\tau < 1$. This proves

$$\|\phi(x_1) - \phi(x_2)\|_{C^\alpha(I_{\tau_3}, C^2(Y))} + \|c_s(x_1) - c_s(x_2)\|_{C^\alpha(I_{\tau_3}, C^2(Y))} \le c\|C^{\mathcal{V}}(x_1) - C^{\mathcal{V}}(x_2)\|_{C(I_{\tau_3})},$$

with a constant $c > 0$ depending only on the initial, boundary and macroscopic coupling data. The right hand side tends to zero for $|x_1 - x_2| \to 0$, since $C^{\mathcal{V}}$ is continuous with respect to x. It follows that ϕ, c_s and, due to Lemmata 3.4, 3.7, also $\hat{v}$, $\hat{p}$ and $\hat{u}$ are continuous with respect to x.
Take the maximum with respect to $x \in S_0$ on both sides of the a priori estimate (3.41) to prove (3.42). □

Lemma 3.17 (Continuity with respect to the coupling data)**.** *Suppose $C_1^{\mathcal{V}}, C_2^{\mathcal{V}} \in C(I_{\tau_3} \times S_0)$ and denote by $\phi_i, c_{s,i}, \hat{u}_i, \hat{v}_i$ and $\hat{p}_i$, $i = 1, 2$, the corresponding solutions of the microscopic problem (2.29) – (2.38). These solutions depend locally Lipschitz continuous on $C_1^{\mathcal{V}}$ and $C_2^{\mathcal{V}}$, i.e. if $\|C_i^{\mathcal{V}}\|_{C(I_{\tau_3} \times S_0)} \le R$, for some $R > 0$, then*

$$\begin{aligned}
&\|\phi_1 - \phi_2\|_{C(S_0, C^{1,2+2\alpha}(I_{\tau_3} \times Y))} + \|c_{s,1} - c_{s,2}\|_{C(S_0, C^{1,2+2\alpha}(I_{\tau_3} \times Y))} + \|\hat{v}_1 - \hat{v}_2\|_{C(I_{\tau_3} \times S_0, W^2_{r,\mathrm{per}}(\hat{Q}_{lK}))} \\
&\quad + \|\hat{p}_1 - \hat{p}_2\|_{C(I_{\tau_3} \times S_0, W^1_{r,\mathrm{per}}(\hat{Q}_{lK}))} + \|\hat{u}_1 - \hat{u}_2\|_{C(I_{\tau_3} \times S_0, W^2_{r,\mathrm{per}}(\hat{Q}_s))} \\
&\quad \le c\|C_1^{\mathcal{V}} - C_2^{\mathcal{V}}\|_{C(I_{\tau_3} \times S_0)},
\end{aligned} \tag{3.44}$$

with a constant $c > 0$ depending on R.

Proof. Consider first fixed $x \in S_0$. Analogously to the proof of Lemma 3.16 it holds

$$\|\phi_1(x) - \phi_2(x)\|_{C^\alpha(I_{\tau_3}, C^2(Y))} + \|c_{s,1}(x) - c_{s,2}(x)\|_{C^\alpha(I_{\tau_3}, C^2(Y))} \le c\|C_1^{\mathcal{V}}(x) - C_2^{\mathcal{V}}(x)\|_{C(I_{\tau_3})},$$

with a constant $c > 0$ depending only on the initial, boundary and macroscopic coupling data. The continuity estimates of Lemmata 3.4 and 3.7 then imply

$$\begin{aligned}
&\|\phi_1(x) - \phi_2(x)\|_{C^{1,2+2\alpha}(I_{\tau_3} \times Y)} + \|c_{s,1}(x) - c_{s,2}(x)\|_{C^{1,2+2\alpha}(I_{\tau_3} \times Y)} \\
&\quad + \|\hat{v}_1(x) - \hat{v}_2(x)\|_{C(I_{\tau_3}, W^2_{r,\mathrm{per}}(\hat{Q}_{lK}))} + \|\hat{p}_1(x) - \hat{p}_2(x)\|_{C(I_{\tau_3}, W^1_{r,\mathrm{per}}(\hat{Q}_{lK}))} \\
&\quad + \|\hat{u}_1(x) - \hat{u}_2(x)\|_{C(I_{\tau_3}, W^2_{r,\mathrm{per}}(\hat{Q}_s))} \\
&\quad \le c\|C_1^{\mathcal{V}}(x) - C_2^{\mathcal{V}}(x)\|_{C(I_{\tau_3})}.
\end{aligned}$$

Taking the maximum with respect to $x \in S_0$ proves (3.44). □

Remark 3.18. *The proofs of the last two Lemmata work also with less regularity assumptions on $C^{\mathcal{V}}$ as for example $C^{\mathcal{V}} \in L_2(S_0, C(I_{\tau_3}))$ and then lead to $\phi \in L_2(S_0, C^{1,2+2\alpha}(I_{\tau_3} \times Y))$ etc. But note, that the spaces $L_2(S_0, C(I_{\tau_3}))$ and $C(I_{\tau_3}, L_2(S_0))$ do not coincide, and it is not clear, how to prove $C^{\mathcal{V}} \in L_2(S_0, C(I_{\tau_3}))$ as a solution of the macroscopic problem.*

The only microscopic quantity, which occurs in the macroscopic problem as coupling datum, is the microscopic mean value $\bar{c}_s$. Therefore, the following Lemma, is stated explicity:

Lemma 3.19 (On the microscopic mean value $\bar{c}_s$)**.** *It holds*

$$\|\bar{c}_s\|_{C^1(I_{\tau_3},C(S_0))} \le c\Big(1 + \|C^{\mathcal{V}}\|^2_{C(I_{\tau_3}\times S_0)} + \|\nabla_x V\|^2_{C(I_{\tau_3}\times S_0)} + \|P\|^2_{C(I_{\tau_3}\times S_0)}$$
$$+ \|b\|^2_{C(I_{\tau_3}\times S_0, W_r^{2-1/r}(Y\times\{0\}))} + \|\phi_{ini}\|_{C(S_0,C^{2+2\alpha}(Y))} + \|c_{s,ini}\|^2_{C(S_0,C^{2+2\alpha}(Y))}\Big),$$

and

$$\|\bar{c}_{s,1} - \bar{c}_{s,2}\|_{C^1(I_{\tau_3},C(S_0))} \le c\|C_1^{\mathcal{V}} - C_2^{\mathcal{V}}\|_{C(I_{\tau_3}\times S_0)},$$

with the same constant $c > 0$ as in Lemma 3.17.

Proof. Note that Y does not depend on t and thus

$$\partial_t \bar{c}_s(x,t) = \partial_t \int_Y c_s(x,t,y)\,\mathrm{d}y = \int_Y \partial_t c_s(x,t,y)\,\mathrm{d}y = \overline{\partial_t c_s}(x,t).$$

The statements follow from

$$|\bar{f}(x,t)| = \left|\int_Y f(x,t,y)\,\mathrm{d}y\right| \le \|f(x,t)\|_{C(Y)} \int_Y 1\,\mathrm{d}y, \qquad f \in \{c_s, \partial_t c_s\},$$

and $|Y| = 1$ and estimates (3.42) and (3.44) respectively. □

3.3 The Macroscopic Problem

The macroscopic part of the two scale model consists of the Navier-Stokes equations (2.21) with boundary and initial conditions (2.24), (2.26), (2.28), and the convection-diffusion equation (2.22) with boundary and initial conditions (2.23), (2.25), (2.27). These equations are posed on $I \times Q$, where Q has the form of a container, as introduced in section 2, with bottom S_0 (in particular, Q is a time-independent convex and bounded polyhedron, and S_0 one of its flat faces).

V and P are considered as given solutions of the Navier-Stokes problem. If not stated differently, V is supposed to be an element of $C^\beta(I, C(\overline{Q}))$ throughout this section, with some $\beta > 0$. It remains to investigate the convection-diffusion problem with $\bar{c}_s$ as coupling datum. Existence and uniqueness of a weak solution of the problem $C^{\mathcal{V}} \in L_2(I, H^1(Q))$ with $\partial_t C^{\mathcal{V}} \in L_2(I, H^1(Q)')$ have already been proven in [8]. Unfortunately, these regularity properties for $C^{\mathcal{V}}$ do not suffice for the coupling to the microscopic problem:

- **Space regularity:** Lemma 3.16 supposes $C^{\mathcal{V}}(\cdot,t) \in C(S_0)$, see also Remark 3.18. If $C^{\mathcal{V}}(\cdot,t) \in H^1(Q)$, then $C^{\mathcal{V}}(\cdot,t) \in H^{1/2}(S_0)$ in the usual trace sense, and $H^{1/2}(S_0)$ is not embedded into $C(S_0)$.
- **Time regularity:** The existence of microscopic solutions is proven in section 3.2 in spaces of continuous functions in time, because uniform in time bounds for $\|\phi(t)\|_{C^2(Y)}$ are needed there. This is proven under the condition that also the coupling quantity $C^{\mathcal{V}}$ is continuous in time, i.e. $C^{\mathcal{V}}(x,\cdot) \in C(I)$. In fact, if $C^{\mathcal{V}} \in L_2(I, H^1(Q))$ with $\partial_t C^{\mathcal{V}} \in L_2(I, H^1(Q)')$, then $C^{\mathcal{V}} \in C(I, L_2(Q))$, see [25], Lemma 11.4, p.383, but $C^{\mathcal{V}} \in C(I \times S_0)$ is needed.

So, further regularity studies are necessary. The main limiting factors for the space regularity are the smoothness of $\partial\Omega$ and especially the mixed (Robin-Neumann) boundary conditions (2.23), (2.25). A solution in $W_r^2(Q)$ or even $C^2(Q)$ or $C^{2+\alpha}(Q)$ can not be expected. The subsequent discussion pursues the following strategy:

Aim:

Prove $C^{\mathcal{V}} \in C(I, W_r^1(Q))$, with $r > 3$. Then $C^{\mathcal{V}} \in C(I \times S_0)$ due to the embedding $W_r^1(Q) \hookrightarrow C(\overline{Q})$. In order to do this:

- Consider the corresponding stationary problem

$$-D^{\mathcal{V}}\Delta C^{\mathcal{V}} + V\cdot\nabla C^{\mathcal{V}} = 0, \qquad \text{in } Q, \qquad D^{\mathcal{V}}\frac{\partial C^{\mathcal{V}}}{\partial n} = \begin{cases} \dfrac{\bar{c}_s}{\tau_s} - \dfrac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}}, & \text{on } S_0,\\ 0, & \text{on } \partial Q\setminus S_0. \end{cases} \tag{3.45}$$

Prove the existence of a unique weak solution $C^{\mathcal{V}} \in W^1_r(Q)$, see Theorems 3.24 and 3.25. The weak formulation (see problem 3.22 on page 27) of (3.45) can be written as

$$-AC^{\mathcal{V}} = \ell_{c_s},$$

with ℓ_{c_s} depending on c_s and an operator

$$A(t)\colon W^1_r(Q) \to \big(W^1_{r'}(Q)\big)', \qquad \text{with} \quad \frac{1}{r} + \frac{1}{r'} = 1, \tag{3.46}$$

defined in (3.48). $A = A(t)$ depends on t, because V depends on t.

- Study the eigenvalue problem
$$-A(t)C^{\mathcal{V}} + \lambda C^{\mathcal{V}} = \ell,$$
for fixed $t \in I$, and prove an estimate for the resolvent $R(\lambda, A)$ in order to show that, for any $t \in I$, $A(t)$ is sectorial, see Lemmata 3.26 and 3.27. Then, $A(t)$ is the generator if an analytic semigroup, see [20].

- Use semigroup theory to prove the existence and uniqueness of a solution $C^{\mathcal{V}} \in C(I, W^1_r(Q))$ of
$$\partial_t C^{\mathcal{V}} = A(t)C^{\mathcal{V}} + \ell_{c_s}, \qquad \text{in} \quad I = [0,T], \qquad C^{\mathcal{V}}(0) = C^{\mathcal{V}}_{ini},$$
(see Theorem 3.29), which is a reformulation of the convection-diffusion problem (2.22), (2.23), (2.25), (2.27).

Remark 3.20. *In the case, where the stationary problem* (3.45) *has smooth solutions in* $W^2_r(Q)$ *or* $C^{2+\alpha}(Q)$*, all of the three just mentioned items are covered by well-known literature as for example [20]. The case of non-smooth solutions (of the stationary problem) is less considered in the literature. We consider Theorem 3.29 also as a contribution to the general regularity theory of parabolic partial differential equations.*

The stationary problem

Suppose $1 < r, r' < \infty$ with $\frac{1}{r} + \frac{1}{r'} = 1$, $w \in W^1_{r'}(Q)$. Multiply the first equation in (3.45) by w and integrate by parts to get

$$\int_Q \big(D^{\mathcal{V}} \nabla C^{\mathcal{V}} \cdot \nabla w + V \cdot \nabla C^{\mathcal{V}} w\big)\,\mathrm{d}x + \int_{S_0} \frac{1}{\tau^{\mathcal{V}}} C^{\mathcal{V}} w \,\mathrm{d}s = \int_{S_0} \frac{1}{\tau_s} \bar{c}_s w \,\mathrm{d}s.$$

Using $\operatorname{div} V = 0$ in Q and $V \cdot n = 0$ on ∂Q, the convection term can be rewritten as follows:

$$\int_Q V \cdot \nabla C^{\mathcal{V}} w \,\mathrm{d}x = \int_{\partial Q} C^{\mathcal{V}} w \underbrace{V \cdot n}_{=0} \mathrm{d}s - \int_Q \left(C^{\mathcal{V}} w \underbrace{\operatorname{div} V}_{=0} + C^{\mathcal{V}} V \cdot \nabla w \right) \mathrm{d}x = - \int_Q C^{\mathcal{V}} V \cdot \nabla w \,\mathrm{d}x$$

Define

$$a(C^{\mathcal{V}}, w) := \int_Q \big(D^{\mathcal{V}} \nabla C^{\mathcal{V}} \cdot \nabla w - C^{\mathcal{V}} V \cdot \nabla w\big)\,\mathrm{d}x + \int_{S_0} \frac{1}{\tau^{\mathcal{V}}} C^{\mathcal{V}} w \,\mathrm{d}s, \qquad \langle \ell_{c_s}, w\rangle := \int_{S_0} \frac{1}{\tau_s} \bar{c}_s w \,\mathrm{d}s, \tag{3.47}$$

where $\langle \cdot, \cdot \rangle$ denotes the dual pairing on $\big(W^1_{r'}(Q)\big)' \times W^1_{r'}(Q)$. For $\bar{c}_s \in C(S_0)$, this notation makes sense:

Lemma 3.21. *Suppose* $\bar{c}_s \in C(S_0)$ *and* $1 \le r' \le \infty$*. Then,* $\ell_{c_s} \in \big(W^1_{r'}(Q)\big)'$ *with*

$$\|\ell_{c_s}\|_{(W^1_{r'}(Q))'} \le c \|\bar{c}_s\|_{C(S_0)}.$$

The operator A in (3.46) is defined by

$$A\colon W^1_r(Q) \to \big(W^1_{r'}(Q)\big)' \colon \quad AC^{\mathcal{V}} := -a(C^{\mathcal{V}}, \cdot). \tag{3.48}$$

Note that $A = A(t)$ depends on time, since V depends on time. A **weak formulation** for (3.45) is:

Problem 3.22. *Find $C^{\mathcal{V}} \in W^1_r(Q)$ such that $a(C^{\mathcal{V}}, w) = \langle \ell_{c_s}, w\rangle$, for all $w \in W^1_{r'}(Q)$.*

The continuity of a is a consequence of Hölder's inequality and the continuity of the trace operator:

Lemma 3.23. *The bilinear form $a\colon W^1_r(Q) \times W^1_{r'}(Q) \to \mathbb{R}$ is continuous.*

There is a unique weak solution for the stationary convection-diffusion problem in the Hilbert-space case:

Theorem 3.24 (Solvability of the stationary problem in $H^1(Q)$)**.** *Suppose $\bar{c}_s \in C(S_0)$, $D^{\mathcal{V}}, \tau^{\mathcal{V}} > 0$ and $r = r' = 2$. Then, there is a unique solution of Problem 3.22 in $H^1(Q)$.*

Proof. In order to apply the Lax-Milgram Theorem, it remains to prove (in addition to the Lemmata 3.21 and 3.23), that the bilinear form a is $H^1(Q)$-elliptic, i.e. there is a constant $c > 0$ such that

$$a(C^{\mathcal{V}}, C^{\mathcal{V}}) \geq c\|C^{\mathcal{V}}\|^2_{H^1(Q)}.$$

Note first, that for $w = C^{\mathcal{V}}$, the convection term cancels, due to $\operatorname{div} V = 0$ and $V \cdot n = 0$:

$$\int_Q V \cdot \nabla C^{\mathcal{V}} C^{\mathcal{V}} \,\mathrm{d}x = \int_Q V \cdot \frac{1}{2}\nabla |C^{\mathcal{V}}|^2 \,\mathrm{d}x = \int_{\partial Q} \frac{1}{2}|C^{\mathcal{V}}|^2 \underbrace{V \cdot n}_{=0} \,\mathrm{d}s - \int_Q \frac{1}{2} C^{\mathcal{V}} \underbrace{\operatorname{div} V}_{=0} \,\mathrm{d}x = 0.$$

So, $a(C^{\mathcal{V}}, C^{\mathcal{V}})$ reduces to

$$a(C^{\mathcal{V}}, C^{\mathcal{V}}) = \int_Q D^{\mathcal{V}} \left|\nabla C^{\mathcal{V}}\right|^2 \mathrm{d}x + \int_{S_0} \frac{1}{\tau^{\mathcal{V}}} \left|C^{\mathcal{V}}\right|^2 \mathrm{d}s. \tag{3.49}$$

In fact, $\|C^{\mathcal{V}}\|_a := \left(\int_Q D^{\mathcal{V}} \left|\nabla C^{\mathcal{V}}\right|^2 \mathrm{d}x + \int_{S_0} \frac{1}{\tau^{\mathcal{V}}} \left|C^{\mathcal{V}}\right|^2 \mathrm{d}s\right)^{\frac{1}{2}}$ defines a norm on $H^1(Q)$ which is equivalent to the usual $H^1(Q)$-norm, which can be proven as in the proof of Theorem 21.A in [31], pp.247-248. This proves $H^1(Q)$-ellipticity of a. □

For the discussion of the regularity of the solution, the mixed boundary value problem (3.45) can be rewritten as a Neumann problem, as described in the proof of the following theorem:

Theorem 3.25 (Regularity/Solvability of the stationary problem in $W^1_r(Q)$)**.** *Suppose $\bar{c}_s \in C(S_0)$ and $C^{\mathcal{V}} \in H^1(Q)$ is the unique solution of Problem 3.22 for $r = r' = 2$. Then $C^{\mathcal{V}} \in W^1_r(Q)$ for any $r \geq 2$. Furthermore, $C^{\mathcal{V}}$ is the unique solution of Problem 3.22 for any $r \geq 2$.*

Proof. Suppose in the following $r \geq 2$, $\frac{1}{r} + \frac{1}{r'} = 1$.
The weak formulation in Problem 3.22 is equivalent to the weak formulation of the following Neumann problem:

$$-\Delta C^{\mathcal{V}} = F(C^{\mathcal{V}}), \quad \text{in } Q, \qquad \frac{\partial C^{\mathcal{V}}}{\partial n} = 0, \quad \text{on } \partial Q,$$

with

$$\langle F(C^{\mathcal{V}}), w\rangle := \int_Q C^{\mathcal{V}} V \cdot \nabla w \,\mathrm{d}x - \int_{S_0} \frac{1}{\tau^{\mathcal{V}}} C^{\mathcal{V}} w \,\mathrm{d}s + \langle \ell_{c_s}, w\rangle. \tag{3.50}$$

If $F(C^{\mathcal{V}}) \in \left(W^1_{r'}(Q)\right)'$, then the weak solution of the above Neumann problem, and therefore the solution of problem 3.22, belongs to $W^1_r(Q)$, thanks to [21], Theorem 8.3.10, p.377.
In order to prove $F(C^{\mathcal{V}}) \in \left(W^1_{r'}(Q)\right)'$, suppose $w \in W^1_{r'}(Q)$ and study every term in (3.50) separately:

- $C^{\mathcal{V}} \in H^1(Q)$ implies $C^{\mathcal{V}} \in L_6(Q)$, due to the Sobolev embedding. Due to Hölder's inequality, the volume integral is finite, if $\nabla w \in L_{\frac{6}{5}}(Q)$, i.e. for $r' \geq \frac{6}{5}$.
- $C^{\mathcal{V}} \in H^1(Q)$ implies $C^{\mathcal{V}} \in H^{\frac{1}{2}}(S_0)$ in the trace sense, and $H^{\frac{1}{2}}(S_0) \hookrightarrow L_4(S_0)$. So the boundary integral in (3.50) is finite, if $w \in L_{\frac{4}{3}}(S_0)$, due to Hölder's inequality. $w \in W^1_{r'}(Q)$ implies $w \in W^{1-\frac{1}{r'}}_{r'}(S_0)$ and $W^{1-\frac{1}{r'}}_{r'}(S_0) \hookrightarrow L_{\frac{4}{3}}(S_0)$ for $r' \geq \frac{6}{5}$.
- The last term is finite for any $r' \geq 1$, due to Lemma 3.21.

It follows that $F(C^{\mathcal{V}}) \in \big(W^1_{r'}(Q)\big)'$ for $r' \geq \frac{6}{5}$, and thus $C^{\mathcal{V}} \in W^1_r(Q)$ for $r \leq 6$. This result can be improved by repeating the same arguments, starting from $C^{\mathcal{V}} \in W^1_6(Q)$ instead of $C^{\mathcal{V}} \in H^1(Q)$. Suppose again $w \in W^1_{r'}(Q)$. Then:

- $C^{\mathcal{V}} \in W^1_6(Q)$ implies $C^{\mathcal{V}} \in L_\infty(Q)$. So the volume integral is finite, if $\nabla w \in L_1(Q)$, which is true for any $r' \geq 1$.
- $C^{\mathcal{V}} \in W^1_6(Q)$ implies $C^{\mathcal{V}} \in W^{\frac{5}{6}}_6(S_0)$ and $W^{\frac{5}{6}}_6(S_0) \hookrightarrow L_\infty(S_0)$. So the boundary integral in (3.50) is finite, if $w \in L_1(S_0)$ which is given for any $r' \geq 1$.

Consequently $C^{\mathcal{V}}$ belongs to $W^1_r(Q)$ and satisfies $a(C^{\mathcal{V}}, w) = \langle \ell_{c_s}, w\rangle$, for all $w \in H^1(Q)$ by assumption. Since $H^1(Q)$ is dense in $W^1_{r'}(Q)$, $C^{\mathcal{V}}$ solves Problem 3.22 for any $r \geq 2$, $\frac{1}{r} + \frac{1}{r'} = 1$.
It is proven now, that a solution for $r = 2$ also is a solution for $r \geq 2$. The converse statement is trivially true. The solution for $r = 2$ is unique, and so is that for $r \geq 2$. ☐

On the resolvent $R(\lambda, A)$

The study of the evolution equation

$$\partial_t C^{\mathcal{V}} = A(t)C^{\mathcal{V}} + \ell_{c_s}$$

is done in the framework of semigroup theory. The abstract theory for parabolic problems considers the situation of a Banach space X and a linear sectorial operator $A\colon D(A) \subset X \to X$ with domain $D(A)$. As special case, $X = L_r(\Omega)$ and $D(A) \subseteq W^2_r(\Omega)$ is treated for example in [20] and [23], and it is proven that several linear elliptic operators of second order are sectorial in this context. These results are not applicable here, because the regularity properties of the solution of the stationary convection-diffusion problem are not good enough. In the following passage, it is proven that the operator $A(t_0)$ from (3.48), for fixed $t_0 \in I$, is sectorial for $X = \big(W^1_{r'}(Q)\big)'$ and $D(A) = W^1_r(Q)$, and generates an analytic semigroup on $\big(W^1_{r'}(Q)\big)'$.
So, consider in the following the operator $A = A(t_0)$ at fixed $t_0 \in I$.

Lemma 3.26. *The resolvent set $\rho(A)$ contains the complex half plane $\{\lambda \in \mathbb{C} :\ \operatorname{Re}\lambda \geq 0\}$.*

Proof. Suppose first $\lambda \in \mathbb{R}$, $\ell \in \big(W^1_{r'}(Q)\big)'$ and consider the equation

$$-AC^{\mathcal{V}} + \lambda C^{\mathcal{V}} = \ell. \tag{3.51}$$

Equation (3.51) is an equation in $\big(W^1_{r'}(Q)\big)'$, so $C^{\mathcal{V}} \in W^1_r(Q)$ is understood as an element of $\big(W^1_{r'}(Q)\big)'$ by setting $\langle C^{\mathcal{V}}, w\rangle := \int_Q C^{\mathcal{V}} w \,\mathrm{d}x$, for all $w \in W^1_{r'}(Q)$. Then (3.51) can be written as

$$a_\lambda(C^{\mathcal{V}}, w) := a(C^{\mathcal{V}}, w) + \lambda \int_Q C^{\mathcal{V}} w \,\mathrm{d}x = \langle \ell, w\rangle, \qquad \forall w \in W^1_{r'}(Q). \tag{3.52}$$

In the Hilbert space case $r = r' = 2$, the bilinear form a_λ is obviously continuous and also $H^1(Q)$-elliptic if $\lambda \geq 0$. Therefore, there exists for each $\ell \in \big(H^1(Q)\big)'$ a unique $C^{\mathcal{V}} \in H^1(Q)$ solving (3.52), due to the Lax-Milgram theorem. A repetition of the arguments in the proof of Theorem 3.25 yields that $C^{\mathcal{V}}$ belongs to $W^1_r(Q)$ and is the unique solution of (3.52) for any $r \geq 2$.
For complex λ the bilinear forms a and a_λ have to be understood as sesquilinear forms:

$$\begin{aligned} a(C^{\mathcal{V}}, w) &= \int_Q \Big(\overline{D^{\mathcal{V}} \nabla C^{\mathcal{V}}} \cdot \nabla w + \overline{C^{\mathcal{V}} V} \cdot \nabla w\Big) \,\mathrm{d}x + \int_{S_0} \overline{\frac{1}{\tau^{\mathcal{V}}} C^{\mathcal{V}}} w \,\mathrm{d}s, \\ a_\lambda(C^{\mathcal{V}}, w) &= a(C^{\mathcal{V}}, w) + \lambda \int_Q \overline{C^{\mathcal{V}}} w \,\mathrm{d}x. \end{aligned}$$

For $r = r' = 2$, the ellipticity condition $\operatorname{Re}\big(a_\lambda(C^{\mathcal{V}}, C^{\mathcal{V}})\big) \geq c\|C^{\mathcal{V}}\|^2_{H^1(Q)}$, on a_λ in the Lax-Milgram theorem (see [2], Theorem 4.2, p.164) is satisfied if $\operatorname{Re}\lambda \geq 0$. It follows, that there exists for each $\ell \in \big(H^1(Q)\big)'$ a unique $C^{\mathcal{V}} \in W^1_r(Q)$ solving (3.52), if $\operatorname{Re}\lambda \geq 0$.

Concluding, it is proven that for $\operatorname{Re}\lambda \geq 0$ the operator $-A + \lambda\mathbf{I} : W_r^1(Q) \to \left(W_{r'}^1(Q)\right)'$, is linear and continuous, due to the continuity of a_λ, and bijective, due to the existence and uniqueness of the solution of (3.52). By the bounded inverse theorem, the inverse $(-A + \lambda\mathbf{I})^{-1} : \left(W_{r'}^1(Q)\right)' \to W_r^1(Q)$, is linear and bounded, i.e. the solution $C^{\mathcal{V}}$ of (3.52) satisfies the a priori estimate

$$\|C^{\mathcal{V}}\|_{W_r^1(Q)} \leq c\|\ell\|_{\left(W_{r'}^1(Q)\right)'}. \tag{3.53}$$

Furthermore, the resolvent operator $R(\lambda, A) = (-A + \lambda\mathbf{I})^{-1}$ belongs to $L(X, X)$, with $X = \left(W_{r'}^1(Q)\right)'$, which implies that $\lambda \in \rho(A)$. □

Lemma 3.27. *For $\lambda \in \mathbb{C}$ with $\operatorname{Re}\lambda \geq 0$, the resolvent $R(\lambda, A)$ satisfies the estimate*

$$\|\lambda R(\lambda, A)\|_{L\left(\left(W_{r'}^1(Q)\right)'\right)} \leq c,$$

with a constant $c > 0$. Thus, the operator $A(t_0)$, for any fixed $t_0 \in I$, is sectorial.

Proof. Consider $\ell \in \left(W_{r'}^1(Q)\right)'$ and suppose that $C^{\mathcal{V}} = R(\lambda, A)\,\ell$ is the corresponding solution of (3.52). Then

$$\begin{aligned}\|\lambda R(\lambda, A)\,\ell\|_{\left(W_{r'}^1(Q)\right)'} &= \|\lambda C^{\mathcal{V}}\|_{\left(W_{r'}^1(Q)\right)'} = \sup_{\substack{w \in W_{r'}^1(Q),\\ \|w\|_{W_{r'}^1(Q)}=1}} \lambda\langle C^{\mathcal{V}}, w\rangle = \sup_{\substack{w \in W_{r'}^1(Q),\\ \|w\|_{W_{r'}^1(Q)}=1}} \left(a_\lambda(C^{\mathcal{V}}, w) - a(C^{\mathcal{V}}, w)\right)\\ &\overset{(3.52)}{\leq} \|\ell\|_{\left(W_{r'}^1(Q)\right)'} + \sup_{\substack{w \in W_{r'}^1(Q),\\ \|w\|_{W_{r'}^1(Q)}=1}} a(C^{\mathcal{V}}, w) \overset{\text{Lemma 3.23}}{\leq} \|\ell\|_{\left(W_{r'}^1(Q)\right)'} + c\|C^{\mathcal{V}}\|_{W_r^1(Q)}\\ &\overset{(3.53)}{\leq} \tilde{c}\|\ell\|_{\left(W_{r'}^1(Q)\right)'}.\end{aligned}$$

Due to [20], Proposition 2.1.11, p.43, A is sectorial. □

The evolution problem

Consider the nonstationary convection-diffusion problem

$$\partial_t C^{\mathcal{V}} = A(t)C^{\mathcal{V}} + \ell_{c_s}, \qquad \text{in} \quad I = [0, T], \qquad C^{\mathcal{V}}(0) = C_{ini}^{\mathcal{V}}. \tag{3.54}$$

The spatial differential operator A is treated in a weak formulation, while the time derivative has to be understood in the classical sense.
Problem (3.54) is a nonautonomous problem, because $A = A(t)$ depends on time. Fortunately, existence and regularity of solutions can be proven, by using a result for the autonomous case, namely Theorem. 4.3.1.(ii) in [20], since the time dependency of A only occurs in its coefficients for lower order terms. A key role plays the following interpolation lemma:

Lemma 3.28. *Suppose $r \geq 2$, $C^{\mathcal{V}} \in C^1(I, \left(W_{r'}^1(Q)\right)') \cap C(I, W_r^1(Q))$. Then $C^{\mathcal{V}} \in C^{\frac{1}{r}}(I, L_r(Q))$ with*

$$\|C^{\mathcal{V}}\|_{C^{\frac{1}{r}}(I, L_r(Q))} \leq c\left(\|C^{\mathcal{V}}\|_{C^1(I, (W_{r'}^1(Q))')} + \|C^{\mathcal{V}}\|_{C(I, W_r^1(Q))}\right).$$

A proof can be found in [16], Lemma 2.16. The exact procedure is explained in the proof of the following theorem, the most important result of this section:

Theorem 3.29 (Existence and uniqueness of a solution of the macroscopic problem)**.** *Suppose $r \geq 2$, $C_{ini}^{\mathcal{V}} \in W_r^1(Q)$, $\bar{c}_s \in C^\beta(I, C(S_0))$ and $V \in C^\beta(I, C(\overline{Q}))$ for some $\beta > 0$. Then, there exists a unique solution $C^{\mathcal{V}} \in C^1(I, \left(W_{r'}^1(Q)\right)') \cap C(I, W_r^1(Q))$ of (3.54) satisfying the a priori estimate*

$$\|C^{\mathcal{V}}\|_{C(I, W_r^1(Q))} + \|C^{\mathcal{V}}\|_{C^1(I, (W_{r'}^1(Q))')} \leq c\left(\|\bar{c}_s\|_{C^\beta(I, C(S_0))} + \|C_{ini}^{\mathcal{V}}\|_{W_r^1(Q)}\right). \tag{3.55}$$

Proof. Assume w.l.o.g. $\beta \leq \frac{1}{r}$. The differential equation in (3.54) can be rewritten as

$$\partial_t C^{\mathcal{V}} = A(0)C^{\mathcal{V}} + (A(t) - A(0))\, C^{\mathcal{V}} + \ell_{c_s}.$$

To shorten the notation during the proof set

$$W = C^1(I, \left(W^1_{r'}(Q)\right)') \cap C(I, W^1_r(Q)), \qquad \|\cdot\|_W := \|\cdot\|_{C(I,W^1_r(Q))} + \|\cdot\|_{C^1(I,(W^1_{r'}(Q))')}.$$

Define $W_0 = \left\{\varphi \in W |\, \varphi(0) = C^{\mathcal{V}}_{ini}\right\}$. Suppose $\widetilde{C^{\mathcal{V}}} \in W_0$ and consider

$$\partial_t C^{\mathcal{V}} = A(0)C^{\mathcal{V}} + (A(t) - A(0))\, \widetilde{C^{\mathcal{V}}} + \ell_{c_s}, \qquad C^{\mathcal{V}}(0) = C^{\mathcal{V}}_{ini}, \tag{3.56}$$

which is an autonomous problem for fixed $\widetilde{C^{\mathcal{V}}}$, with a sectorial operator $A(0)$. Prove that

- for any $\widetilde{C^{\mathcal{V}}} \in W_0$ there exists a unique solution $C^{\mathcal{V}}$ of (3.56) and
- the mapping $\mathcal{F}\colon W_0 \to W_0\colon\ \widetilde{C^{\mathcal{V}}} \mapsto C^{\mathcal{V}}$ has a unique fixed point.

Start by discussing the regularity of the right hand side terms in (3.56):

$$\begin{aligned}\langle (A(t) - A(0))\, \widetilde{C^{\mathcal{V}}}, w\rangle &= \int_Q \widetilde{C^{\mathcal{V}}}\, (V(0) - V(t)) \cdot \nabla w \,\mathrm{d}x \\ &\leq \|V(0) - V(t)\|_{C(Q)} \|\, \widetilde{C^{\mathcal{V}}}\, \|_{L_r(Q)} \|w\|_{W^1_{r'}(Q)}.\end{aligned} \tag{3.57}$$

Due to Lemma 3.28 it is $\widetilde{C^{\mathcal{V}}} \in C^{\frac{1}{r}}(I, L_r(Q))$ and so it follows from (3.57) and from $\beta \leq \frac{1}{r}$ that $(A(t) - A(0))\, \widetilde{C^{\mathcal{V}}} \in C^\beta(I, \left(W^1_{r'}(Q)\right)')$ with

$$\|\, (A(t) - A(0))\, \widetilde{C^{\mathcal{V}}}\, \|_{C^\beta(I,(W^1_{r'}(Q))')} \leq \|V\|_{C^\beta(I,C(\overline{Q}))} \|\, \widetilde{C^{\mathcal{V}}}\, \|_{C^\beta(I,L_r(Q))}.$$

Lemma 3.21 and $\bar{c}_s \in C^\beta(I, C(S_0))$ implies

$$\ell_{c_s} \in C^\beta(I, \left(W^1_{r'}(Q)\right)') \qquad \text{and} \qquad \|\ell_{c_s}\|_{C^\beta(I,(W^1_{r'}(Q))')} \leq c\|\bar{c}_s\|_{C^\beta(I,C(S_0))}.$$

Note furthermore that $W^1_r(Q)$ is dense in $\left(W^1_{r'}(Q)\right)'$, which follows from [1], 3.14, p.65. Thus all the assumptions of [20], Theorem. 4.3.1.(ii) are satisfied and there exists a unique solution $C^{\mathcal{V}} \in W_0$ of (3.56) for any $\widetilde{C^{\mathcal{V}}} \in W_0$ with

$$\begin{aligned}\|C^{\mathcal{V}}\|_W \leq& c\left(\|\, (A(t) - A(0))\, \widetilde{C^{\mathcal{V}}} + \ell_{c_s}\|_{C^\beta(I,(W^1_{r'}(Q))')} + \|C^{\mathcal{V}}_{ini}\|_{W^1_r(Q)}\right) \\ \leq& c\left(\|\, \widetilde{C^{\mathcal{V}}}\, \|_{C^\beta(I,L_r(Q))} + \|\bar{c}_s\|_{C^\beta(I,C(S_0))} + \|C^{\mathcal{V}}_{ini}\|_{W^1_r(Q)}\right).\end{aligned}$$

Problem (3.56) is linear and thus, if $C^{\mathcal{V}}_1, C^{\mathcal{V}}_2 \in W_0$ are the repective solutions for $\widetilde{C^{\mathcal{V}}_1}, \widetilde{C^{\mathcal{V}}_2} \in W_0$, then

$$\partial_t(C^{\mathcal{V}}_1 - C^{\mathcal{V}}_2) = A(0)(C^{\mathcal{V}}_1 - C^{\mathcal{V}}_2) + (A(t) - A(0))\, (\widetilde{C^{\mathcal{V}}_1} - \widetilde{C^{\mathcal{V}}_2}), \qquad (C^{\mathcal{V}}_1 - C^{\mathcal{V}}_2)(0) = 0,$$

with

$$\|C^{\mathcal{V}}_1 - C^{\mathcal{V}}_2\|_W \leq c\|\, \widetilde{C^{\mathcal{V}}_1} - \widetilde{C^{\mathcal{V}}_2}\, \|_{C^\beta(I,L_r(Q))}. \tag{3.58}$$

This and the embedding of W into $C^{\frac{1}{r}}(I, L_r(Q))$, see Lemma 3.28, show that the mapping $\mathcal{F}\colon W_0 \to W_0\colon\ \widetilde{C^{\mathcal{V}}} \mapsto C^{\mathcal{V}}$ exists and is Lipschitz continuous. Reduction of the time interval achieves that

$\mathcal{F}$ is a contraction: Introduce therefore another parameter $\beta < \beta_1 < \frac{1}{r}$ and set $I_\tau = [0, \tau]$ for $\tau > 0$. Then any $\widetilde{C_1^{\mathcal{V}}}, \widetilde{C_2^{\mathcal{V}}} \in W_0$ satisfy

$$\| \widetilde{C_1^{\mathcal{V}}} - \widetilde{C_2^{\mathcal{V}}} \|_{C^\beta(I_\tau, L_r(Q))} \leq c\tau^{\beta_1 - \beta} \| \widetilde{C_1^{\mathcal{V}}} - \widetilde{C_2^{\mathcal{V}}} \|_{C^{\beta_1}(I_\tau, L_r(Q))} \leq c\tau^{\beta_1 - \beta} \| \widetilde{C_1^{\mathcal{V}}} - \widetilde{C_2^{\mathcal{V}}} \|_W, \tag{3.59}$$

due to $\widetilde{C_1^{\mathcal{V}}}(0) = \widetilde{C_2^{\mathcal{V}}}(0)$. Estimates (3.58) and (3.59) with τ small enough prove

$$\|\mathcal{F}(\widetilde{C_1^{\mathcal{V}}}) - \mathcal{F}(\widetilde{C_2^{\mathcal{V}}})\|_W \leq c \| \widetilde{C_1^{\mathcal{V}}} - \widetilde{C_2^{\mathcal{V}}} \|_W,$$

with a constant $c < 1$. Banach's fixed point Theorem implies that there exists a unique solution of (3.54) in W_0 on a possibly reduced time interval I_τ.
It is possible to repeat the procedure, starting from τ as new initial time. In fact, this proves existence and uniqueness of a solution of (3.54) on the time interval $[\tau, 2\tau]$, because the constants in the above estimates can be chosen independently of the initial time, even if this is not obvious: The initial data $C_{ini}^{\mathcal{V}}$ has no influence on the constants but the sectorial operator $A(0)$ in (3.56) has, when applying [20], Theorem. 4.3.1.(ii), see also the remarks in the beginning of chapter 4 in [20], p.122. Fortunately, since the time dependency of A occurs only via V in coefficients of lower order terms and V can be bound uniformly in time, it is possible to give time independent constants in the above estimates, and therefore to choose τ independently of the initial time.
As conclusion, finitely many repetitions of the described method prove existence and uniqueness of a solution of (3.54) in W_0 on the whole time interval I.
The **a priori estimate** (3.55) is proven as follows: Consider again the time interval I_τ, for which $\mathcal{F}$ is a contraction. Denote by $C^{\mathcal{V}}$ the unique solution of (3.54), which is a fixed point of $\mathcal{F}$, and by $\widetilde{C_{ini}^{\mathcal{V}}}$ the function in W_0 which is constant in time, i.e. $\widetilde{C_{ini}^{\mathcal{V}}}(t) = C_{ini}^{\mathcal{V}}$, $\forall t$. Then

$$\begin{aligned} \|C^{\mathcal{V}} - \widetilde{C_{ini}^{\mathcal{V}}}\|_W &= \|\mathcal{F}(C^{\mathcal{V}}) - \mathcal{F}(\widetilde{C_{ini}^{\mathcal{V}}}) + \mathcal{F}(\widetilde{C_{ini}^{\mathcal{V}}}) - \widetilde{C_{ini}^{\mathcal{V}}}\|_W \\ &\leq \|\mathcal{F}(C^{\mathcal{V}}) - \mathcal{F}(\widetilde{C_{ini}^{\mathcal{V}}})\|_W + \|\mathcal{F}(\widetilde{C_{ini}^{\mathcal{V}}}) - \widetilde{C_{ini}^{\mathcal{V}}}\|_W \\ &\leq c\|C^{\mathcal{V}} - \widetilde{C_{ini}^{\mathcal{V}}}\|_W + \|\mathcal{F}(\widetilde{C_{ini}^{\mathcal{V}}}) - \widetilde{C_{ini}^{\mathcal{V}}}\|_W, \end{aligned}$$

with $c < 1$, and therefore

$$\|C^{\mathcal{V}} - \widetilde{C_{ini}^{\mathcal{V}}}\|_W \leq c\|\mathcal{F}(\widetilde{C_{ini}^{\mathcal{V}}}) - \widetilde{C_{ini}^{\mathcal{V}}}\|_W, \tag{3.60}$$

with some $c > 0$. $\widetilde{C_{ini}^{\mathcal{V}}}$ is constant in time and thus

$$\begin{aligned} &\| (A(t) - A(0)) \widetilde{C_{ini}^{\mathcal{V}}} \|_{C^\beta(I_\tau, (W^1_{r'}(Q))')} \leq \|V\|_{C^\beta(I_\tau, C(\overline{Q}))} \| \widetilde{C_{ini}^{\mathcal{V}}} \|_{C^\beta(I_\tau, L_r(Q))} \\ &= \|V\|_{C^\beta(I_\tau, C(\overline{Q}))} \| \widetilde{C_{ini}^{\mathcal{V}}} \|_{C(I_\tau, L_r(Q))} \leq \|V\|_{C^\beta(I_\tau, C(\overline{Q}))} \|C_{ini}^{\mathcal{V}}\|_{W^1_r(Q)}. \end{aligned}$$

$\mathcal{F}(\widetilde{C_{ini}^{\mathcal{V}}})$ is by definition the solution of (3.56) with $\widetilde{C_{ini}^{\mathcal{V}}}$ on the right-hand side, and thus satisfies due to [20], Theorem. 4.3.1.(ii)

$$\begin{aligned} \|\mathcal{F}(\widetilde{C_{ini}^{\mathcal{V}}})\|_W &\leq c \left(\| (A(t) - A(0)) \widetilde{C_{ini}^{\mathcal{V}}} + \ell_{c_s} \|_{C^\beta(I_\tau, (W^1_{r'}(Q))')} + \|C_{ini}^{\mathcal{V}}\|_{W^1_r(Q)} \right) \\ &\leq c \left(\|C_{ini}^{\mathcal{V}}\|_{W^1_r(Q)} + \|\bar{c}_s\|_{C^\beta(I_\tau, C(S_0))} \right). \end{aligned} \tag{3.61}$$

Combining (3.60), (3.61) with $\| \widetilde{C_{ini}^{\mathcal{V}}} \|_W \leq \|C_{ini}^{\mathcal{V}}\|_{W^1_r(Q)}$, leads to

$$\begin{aligned} \|C^{\mathcal{V}}\|_W &\leq \|C^{\mathcal{V}} - \widetilde{C_{ini}^{\mathcal{V}}}\|_W + \| \widetilde{C_{ini}^{\mathcal{V}}} \|_W \leq c\|\mathcal{F}(\widetilde{C_{ini}^{\mathcal{V}}}) - \widetilde{C_{ini}^{\mathcal{V}}}\|_W + \|C_{ini}^{\mathcal{V}}\|_{W^1_r(Q)} \\ &\leq c \left(\|\mathcal{F}(\widetilde{C_{ini}^{\mathcal{V}}})\|_W + \| \widetilde{C_{ini}^{\mathcal{V}}} \|_W \right) + \|C_{ini}^{\mathcal{V}}\|_{W^1_r(Q)} \leq c \left(\|\bar{c}_s\|_{C^\beta(I_\tau, C(S_0))} + \|C_{ini}^{\mathcal{V}}\|_{W^1_r(Q)} \right). \end{aligned} \tag{3.62}$$

Estimate (3.62) is valid on the reduced time interval I_τ. In particular it implies

$$\|C^{\mathcal{V}}(\tau)\|_{W^1_r(Q)} \le c\left(\|\bar{c}_s\|_{C^\beta(I_\tau,C(S_0))} + \|C^{\mathcal{V}}_{ini}\|_{W^1_r(Q)}\right).$$

Therefore, an iteration of these arguments, replacing $C^{\mathcal{V}}_{ini}$ by $C^{\mathcal{V}}(\tau)$ proves (3.55). □

The coupling to the microscopic problem is linear, and thus:

Lemma 3.30 (Continuity with respect to the coupling data)**.** *Suppose* $\bar{c}_{s,1}, \bar{c}_{s,2} \in C^\beta(I, C(S_0))$*, for some* $\beta > 0$ *and denote by* $C^{\mathcal{V}}_1, C^{\mathcal{V}}_2$ *the corresponding solutions of* (3.54)*. Then*

$$\|C^{\mathcal{V}}_1 - C^{\mathcal{V}}_2\|_{C(I,W^1_r(Q))} + \|C^{\mathcal{V}}_1 - C^{\mathcal{V}}_2\|_{C^1(I,(W^1_{r'}(Q))')} \le c\|\bar{c}_{c,1} - \bar{c}_{s,2}\|_{C^\beta(I,C(S_0))}. \tag{3.63}$$

3.4 Micro-Macro-Coupling: Proof of the Main Result

After investigating the microscopic part of the model in section 3.2 and the macroscopic part in section 3.3, their coupling can now be discussed. The most important results of the previous sections are shortly recapitulated here:
For given $C^{\mathcal{V}} \in C(I \times S_0)$ there exists locally in time a unique solution of the microscopic part of the problem (2.29) – (2.38), see Theorem 3.15. This microscopic solution satisfies in particular $\bar{c}_s \in C^1(I_{\tau_3}, C(S_0))$, with τ_3 from Theorem 3.15, and

$$\begin{aligned}\|\bar{c}_s\|_{C^1(I_{\tau_3},C(S_0))} \le c\Big(1 &+ \|C^{\mathcal{V}}\|^2_{C(I_{\tau_3}\times S_0)} + \|\nabla_x V\|^2_{C(I_{\tau_3}\times S_0)} + \|P\|^2_{C(I_{\tau_3}\times S_0)} \\ &+ \|b\|^2_{C(I_{\tau_3}\times S_0, W^{2-1/r}_r(\tilde{\Gamma}))} + \|\phi_{ini}\|_{C(S_0,C^{2+2\alpha}(Y))} + \|c_{s,ini}\|^2_{C(S_0,C^{2+2\alpha}(Y))}\Big).\end{aligned} \tag{3.64}$$

Furthermore, $\bar{c}_s$ depends locally Lipschitz continuous on $C^{\mathcal{V}}$, i.e. if $C^{\mathcal{V}}_1, C^{\mathcal{V}}_2 \le R$, then

$$\|\bar{c}_{s,1} - \bar{c}_{s,2}\|_{C^1(I_{\tau_3},C(S_0))} \le c\|C^{\mathcal{V}}_1 - C^{\mathcal{V}}_2\|_{C(I_{\tau_3}\times S_0)}, \tag{3.65}$$

with a constant c depending on R, see Lemma 3.17.
Conversely, for given $\bar{c}_s \in C^\beta(I, C(S_0))$, with some $\beta > 0$, there exists a unique solution $C^{\mathcal{V}} \in C^1(I, \left(W^1_{r'}(Q)\right)') \cap C(I, W^1_r(Q))$ of the macroscopic problem (2.22), (2.23), (2.25), (2.27), with $r \ge 2$, depending continuously on $\bar{c}_s$ and satisfying

$$\|C^{\mathcal{V}}\|_{C(I,W^1_r(Q))} + \|C^{\mathcal{V}}\|_{C^1(I,(W^1_{r'}(Q))')} \le c\left(\|\bar{c}_s\|_{C^\beta(I,C(S_0))} + \|C^{\mathcal{V}}_{ini}\|_{W^1_r(Q)}\right), \tag{3.66}$$

and

$$\|C^{\mathcal{V}}_1 - C^{\mathcal{V}}_2\|_{C(I,W^1_r(Q))} + \|C^{\mathcal{V}}_1 - C^{\mathcal{V}}_2\|_{C^1(I,(W^1_{r'}(Q))')} \le c\|\bar{c}_{c,1} - \bar{c}_{s,2}\|_{C^\beta(I,C(S_0))}, \tag{3.67}$$

see Theorem 3.29 and Lemma 3.30.
On this basis relies the proof of the main result of this paper:

Proof of Theorem 3.1. Consider the time interval $I_\tau = [0, \tau]$ and suppose that τ is small enough to garantee the existence of a solution of the microscopic problem on I_τ, i.e. $\tau \le \tau_3$, compare Theorem 3.15. Note that for $r_2 > 3$, the space $W^1_{r_2}(Q)$ is continuously embedded into $C(\overline{Q})$, and thus

$$C^{\mathcal{V}} \in C(I_\tau, W^1_{r_2}(Q)) \implies C^{\mathcal{V}} \in C(I_\tau \times \overline{Q}) \implies C^{\mathcal{V}}|_{S_0} \in C(I_\tau \times S_0).$$

Define the solution operators

$$\begin{aligned}\mathcal{L}_{\text{micro}}&\colon C(I_\tau \times \overline{Q}) \quad\;\; \to C^1(I_\tau, C(S_0))\colon C^{\mathcal{V}} \mapsto \bar{c}_s,\\ \mathcal{L}_{\text{macro}}&\colon C^\beta(I_\tau, C(S_0)) \to C(I_\tau \times \overline{Q}) \quad\;\; \colon \bar{c}_s \mapsto C^{\mathcal{V}},\end{aligned}$$

and their composition

$$\mathcal{L} := \mathcal{L}_{\text{macro}} \circ \mathcal{L}_{\text{micro}}\colon C(I_\tau \times \overline{Q}) \to C(I_\tau \times \overline{Q})\colon\; \widetilde{C^{\mathcal{V}}} \mapsto C^{\mathcal{V}}.$$

For $\bar{c}_s \in C^1(I_\tau, C(S_0))$ it is

$$\|\bar{c}_s\|_{C(I_\tau\times S_0)} = \max_{t\in I_\tau} \|\bar{c}_s(t) - \bar{c}_{s,ini} + \bar{c}_{s,ini}\|_{C(S_0)} \le \tau \|\bar{c}_s\|_{C^1(I_\tau,C(S_0))} + \|\bar{c}_{s,ini}\|_{C(S_0)},$$

and thus

$$\begin{aligned} \|\bar{c}_s\|_{C^\beta(I_\tau,C(S_0))} &= \|\bar{c}_s\|_{C(I_\tau\times S_0)} + \sup_{t_1\neq t_2\in I_\tau} \frac{\|\bar{c}_s(t_1) - \bar{c}_s(t_2)\|_{C(S_0)}}{|t_1 - t_2|^\beta} \\ &\le c\left(\tau^{1-\beta}\|\bar{c}_s\|_{C^1(I_\tau,C(S_0))} + \|\bar{c}_{s,ini}\|_{C(S_0)}\right). \end{aligned} \tag{3.68}$$

For $\widetilde{C^\mathcal{V}} \in C(I_\tau \times \overline{Q})$, set $C^\mathcal{V} := \mathcal{L}(\widetilde{C^\mathcal{V}})$. Estimates (3.64) and (3.66), combined with (3.68) and the continuous embedding $C(I_\tau, W^1_{r_2}(Q)) \hookrightarrow C(I_\tau \times \overline{Q})$ imply

$$\begin{aligned} \|C^\mathcal{V}\|_{C(I_\tau\times\overline{Q})} &\le c\|C^\mathcal{V}\|_{C(I_\tau,W^1_{r_2}(Q))} \le c\left(\|\bar{c}_s\|_{C^\beta(I_\tau,C(S_0))} + \|C^\mathcal{V}_{ini}\|_{W^1_{r_2}(Q)}\right) \\ &\le c\left(\tau^{1-\beta}\|\bar{c}_s\|_{C^1(I_\tau,C(S_0))} + \|\bar{c}_{s,ini}\|_{C(S_0)} + \|C^\mathcal{V}_{ini}\|_{W^1_{r_2}(Q)}\right) \\ &\le c_1(V,P,b,C^\mathcal{V}_{ini},\phi_{ini},c_{s,ini}) + c_2\tau^{1-\beta}\|\widetilde{C^\mathcal{V}}\|^2_{C(I_\tau\times\overline{Q})}, \end{aligned} \tag{3.69}$$

with a constant $c_2 > 0$ and

$$\begin{aligned} c_1(V,P,b,C^\mathcal{V}_{ini},\phi_{ini},c_{s,ini}) = c\Big(1 &+ \|\nabla_x V\|^2_{C(I_{\tau_3}\times S_0)} + \|P\|^2_{C(I_{\tau_3}\times S_0)} + \|b\|^2_{C(I_{\tau_3}\times S_0, W^{2-1/r_1}_{r_1}(\tilde{\Gamma}))} \\ &+ \|\phi_{ini}\|_{C(S_0,C^{2+2\alpha}(Y))} + \|c_{s,ini}\|^2_{C(S_0,C^{2+2\alpha}(Y))} + \|C^\mathcal{V}_{ini}\|_{W^1_{r_2}(Q)}\Big). \end{aligned} \tag{3.70}$$

Choose $M_0 := 2c_1$ and define

$$B_\tau = \left\{C^\mathcal{V} \in C(I_\tau\times\overline{Q}) \;\middle|\; \|C^\mathcal{V}\|_{C(I_\tau\times\overline{Q})} \le M_0,\ C^\mathcal{V}(x,0) = C^\mathcal{V}_{ini}(x),\ \forall x\in\overline{Q}\right\}.$$

Then, estimate (3.69) and $M_0 = 2c_1$ imply that $\mathcal{L}$ maps B_τ into itself as long as

$$c_2\tau^{1-\beta}M_0^2 \le \frac{M_0}{2} \qquad \Longleftrightarrow \qquad \tau \le \left(\frac{1}{2M_0}\right)^{\frac{1}{1-\beta}}.$$

In order to apply Banach's fixed point theorem on $\mathcal{L}\colon B_\tau \to B_\tau$, combine estimates (3.65) and (3.67) to get

$$\|C^\mathcal{V}_1 - C^\mathcal{V}_2\|_{C(I_\tau\times\overline{Q})} \le c_3\tau^{1-\beta}\|\widetilde{C^\mathcal{V}_1} - \widetilde{C^\mathcal{V}_2}\|_{C(I_\tau\times\overline{Q})},$$

with a constant c_3 depending on M_0. Therefore, for

$$\tau_0 := \min\left\{\left(\frac{1}{2M_0}\right)^{\frac{1}{1-\beta}}, \left(\frac{1}{2c_3}\right)^{\frac{1}{1-\beta}}\right\},$$

the operator $\mathcal{L}\colon B_{\tau_0} \to B_{\tau_0}$ is a strict contraction and, thus, has a unique fixed point $C^\mathcal{V} \in B_{\tau_0}$.
The existence and regularity results 3.15, 3.16 and 3.29 prove that $C^\mathcal{V}$ and the corresponding microscopic solution (ϕ, c_s, v, p, u) solves the fully coupled two scale model and that in fact

$$C^\mathcal{V} \in C^1\Big(I, \big(W^1_{r_2'}(Q)\big)'\Big) \cap C\Big(I, W^1_{r_2}(Q)\Big).$$

Uniqueness follows as in the proof of Theorem 3.15. □

4 Convergence of the Fixed Point Iteration

In the following, an iterative solving procedure for the two scale model of section 2 is proposed. It can be a basis for both - analysis and numerics. Actually, the strategy of the proof of the main solvability result (Theorem 3.1) in section 3 reflects the following iteration. Conversely, the results of section 3 substantiate the iteration and even ensure its convergence, see Theorem 4.1. All of its assumptions are verified in section 3. Both, the proof of the convergence of the iteration and that of existence and uniqueness of solutions of the two scale model are based on Banach's Fixed Point Theorem.
The macroscopic velocity V and the macroscopic pressure P can be computed in advance since the Navier–Stokes system decouples from the rest of the model equations. The subsequent iterative procedure consists in fact of two encapsulated iterations, see Figure 7: The remaining macroscopic convection–diffusion equation and the coupled microscopic problem (composed of phase field, Stokes and Elasticity system) are solved in turns (outer iteration) where in each step, the microscopic problem is again solved iteratively (inner iteration).
More precisely: Denote by $\mathcal{S}_{\text{Stokes}}$, $\mathcal{S}_{\text{elastic}}$ and $\mathcal{S}_{\text{phasefield}}$ the solution operators of the single microscopic problems, defined in section 3.2.4, and by $\mathcal{L}_{\text{micro}}$ and $\mathcal{L}_{\text{macro}}$ solution operators for the coupled microscopic problem and the macroscopic problem respectively, see section 3.4.
Then, the iteration reads:

1. Solve the decoupled macroscopic Navier–Stokes system (2.21), (2.24), (2.26), (2.28) in the domain $I \times Q$. Get V and P.
2. Choose the initial volume concentration, surface concentration and phase field as functions, which are constant in time, by setting $C_0^{\mathcal{V}}(t) \equiv C_{ini}^{\mathcal{V}}$, $c_{s,0}(t) \equiv c_{s,ini}$ and $\phi_0(t) \equiv \phi_{ini}$, for all $t \in I$.
3. Choose a tolerance $\texttt{tol} > 0$, in order to set an abort criterion for the inner iteration.
4. Solve the microscopic equations, with macroscopic coupling datum $C_0^{\mathcal{V}}$, by an encapsulated iteration procedure:
   (a) Set $\phi^0 := \phi_0$ and $c_s^0 := c_{s,0}$. Calculate $(v^0, p^0) := \mathcal{S}_{\text{Stokes}}(\phi^0, c_s^0)$ as solutions of the microscopic Stokes–system (2.29), (2.30), (2.31).
   (b) Solve the microscopic elasticity system (2.33), (2.34), (2.35) with data v^0, p^0 and ϕ^0 in order to get $u^0 := \mathcal{S}_{\text{elastic}}(v^0, p^0, \phi^0)$.
   (c) Calculate the new quantities $(\phi^1, c_s^1) := \mathcal{S}_{\text{phasefield}}(u^0)$ from the system (2.36), (2.37), (2.38) with coupling datum u^0.
   (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 $\|(\phi^N, c_s^N) - \mathcal{L}_{\text{micro}}(C_0^{\mathcal{V}})\| < \texttt{tol}$.
5. Set $c_{s,1} := c_s^N$. Solve the macroscopic convection–diffusion problem (2.22), (2.23), (2.25), (2.27) to get $C_1^{\mathcal{V}} := \mathcal{L}_{\text{macro}}(c_{s,1})$.
6. Restart in 4. with data $C_1^{\mathcal{V}}$, $c_{s,1}$ and $\phi_1 := \phi^N$ instead of $C_0^{\mathcal{V}}$, $c_{s,0}$ and $\phi_0 \ldots$

The above iteration is meaningful, since the mentioned solution operators exist, due to the results in section 3. Furthermore, the fixed point operators

$$\mathcal{S} := \mathcal{S}_{\text{phasefield}} \circ \mathcal{S}_{\text{elastic}} \circ \mathcal{S}_{\text{Stokes}} \colon \qquad (\tilde{\phi}, \tilde{c_s}) \mapsto (\phi, c_s),$$
$$\mathcal{L} := \mathcal{L}_{\text{macro}} \circ \mathcal{L}_{\text{micro}} \colon \qquad \tilde{C^{\mathcal{V}}} \mapsto C^{\mathcal{V}},$$

are investigated there (see again sections 3.2.4 and 3.4), and it is shown that the assumptions of Banach's Fixed Point Theorem are satisfied for both. In particular, they are strict contractions, that is, that there are numbers $0 \leq k_1, k_2 < 1$ such that

$$\|\mathcal{S}(\phi, c_s) - \mathcal{S}(\tilde{\phi}, \tilde{c_s})\|_1 \leq k_1 \|(\phi, c_s) - (\tilde{\phi}, \tilde{c_s})\|_1,$$
$$\|\mathcal{L}(C^{\mathcal{V}}) - \mathcal{L}(\tilde{C^{\mathcal{V}}})\|_2 \leq k_2 \|C^{\mathcal{V}} - \tilde{C^{\mathcal{V}}}\|_2,$$

with norms

$$\|(\phi, c_s)\|_1 = \|\phi\|_{C^\alpha(I, C^2(Y))} + \|c_s\|_{C^\alpha(I, C^2(Y))}, \qquad \|C^{\mathcal{V}}\|_2 = \|C^{\mathcal{V}}\|_{C(I, W^1_{r_2}(Q))} + \|C^{\mathcal{V}}\|_{C^1(I, (W^1_{r_2'}(Q))')}.$$

The connection between the two operators $\mathcal{S}$ and $\mathcal{L}_{\text{micro}}$ is that for fixed $C^{\mathcal{V}}$ and fixed $x \in S_0$, the solution of the microscopic problem $\mathcal{L}_{\text{micro}}(C^{\mathcal{V}})(x)$ is a fixed point of $\mathcal{S}$.
Convergence of the above iteration can be proven as follows:

Theorem 4.1 (Convergence of the Iteration)**.** *Suppose that $\mathcal{L}_{\text{macro}}$ is Lipschitz continuous with Lipschitz constant L and that $\mathcal{S}$ and $\mathcal{L}$ satisfy the assumptions of Banach's Fixed Point Theorem. Denote by $C^{\mathcal{V}}_*$ the unique fixed point of $\mathcal{L}$ which corresponds to the unique solution of the two scale model. Then*

$$\|C^{\mathcal{V}}_n - C^{\mathcal{V}}_*\|_2 \leq \frac{L \cdot \mathtt{tol}}{1 - k_2} + \frac{k_2^n}{1 - k_2} \|\mathcal{L}(C^{\mathcal{V}}_0) - C^{\mathcal{V}}_0\|_2.$$

Thus, the iteration converges to $C^{\mathcal{V}}_*$ for $\mathtt{tol} \to 0$ and $n \to \infty$.

Proof. Note first, that the inner iteration in the n-th step of the outer iteration can be written as

$$(\phi^0, c_s^0) = (\phi_n, c_{s,n}), \quad (\phi^{k+1}, c_s^{k+1}) = \mathcal{S}(\phi^k, c_s^k), \quad k \in \mathbb{N}_0,$$

which converges to $\mathcal{L}_{\text{micro}}(C^{\mathcal{V}}_n)$, due to Banach's Fixed Point Theorem, since $\mathcal{L}_{\text{micro}}(C^{\mathcal{V}}_n)$ is the unique fixed point of $\mathcal{S}$. Thus, the abort criterion $\|(\phi^N, c_s^N) - \mathcal{L}_{\text{micro}}(C^{\mathcal{V}}_n)\|_1 < \mathtt{tol}$ is reached after finitely many steps for any $n \in \mathbb{N}_0$, and it can be checked using the a priori estimate

$$\|(\phi^N, c_s^N) - \mathcal{L}_{\text{micro}}(C^{\mathcal{V}}_n)\|_1 \leq \frac{k_1^N}{1 - k_1} \|(\phi^1, c_s^1) - (\phi^0, c_s^0)\|_1.$$

Using $\mathcal{L}$, the fixed point iteration $(\tilde{C^{\mathcal{V}}_n})_{n \in \mathbb{N}_0}$, defined by

$$\tilde{C^{\mathcal{V}}_0} := C^{\mathcal{V}}_0, \qquad \tilde{C^{\mathcal{V}}_{n+1}} := \mathcal{L}(\tilde{C^{\mathcal{V}}_n}), \quad n \in \mathbb{N}_0,$$

converges to $C^{\mathcal{V}}_*$, due to Banach's Fixed Point Theorem, and satisfies the a priori estimate

$$\|\tilde{C^{\mathcal{V}}_n} - C^{\mathcal{V}}_*\|_2 \leq \frac{k_2^n}{1 - k_2} \|\mathcal{L}(C^{\mathcal{V}}_0) - C^{\mathcal{V}}_0\|_2. \tag{4.1}$$

In any step of the iteration, it is

$$\begin{aligned} \|C^{\mathcal{V}}_{n+1} - \mathcal{L}(C^{\mathcal{V}}_n)\|_2 &= \|\mathcal{L}_{\text{macro}}(c_{s,n+1}) - \mathcal{L}_{\text{macro}}(\mathcal{L}_{\text{micro}}(C^{\mathcal{V}}_n))\|_2 \\ &\leq L \|\bar{c}_{s,n+1} - \mathcal{L}_{\text{micro}}(C^{\mathcal{V}}_n)\|_{C^1(I, C(S_0))} \leq L \cdot \mathtt{tol}. \end{aligned}$$

It follows that

$$\|C^{\mathcal{V}}_{n+1} - \tilde{C^{\mathcal{V}}_{n+1}}\|_2 \leq \|C^{\mathcal{V}}_{n+1} - \mathcal{L}(C^{\mathcal{V}}_n)\|_2 + \|\mathcal{L}(C^{\mathcal{V}}_n) - \mathcal{L}(\tilde{C^{\mathcal{V}}_n})\|_2 \leq L \cdot \mathtt{tol} + k_2 \|C^{\mathcal{V}}_n - \tilde{C^{\mathcal{V}}_n}\|_2,$$

and finally, due to $C^{\mathcal{V}}_0 = \tilde{C^{\mathcal{V}}_0}$,

$$\|C^{\mathcal{V}}_{n+1} - \tilde{C^{\mathcal{V}}_{n+1}}\|_2 \leq L \cdot \mathtt{tol}(1 + k_2 + \ldots + k_2^n) \leq \frac{L \cdot \mathtt{tol}}{1 - k_2}. \tag{4.2}$$

The combination of (4.1) and (4.2) proves the result. □

5 Conclusion and Outlook

In the paper, a two scale model for liquid phase epitaxy is studied, where elastic effects are included. Based on first results in [11], existence and uniqueness of solutions of the fully coupled model problem is proven as main result via two encapsulated fixed point arguments. Compared to the corresponding model without elasticity, the mathematical structure is much more complicated and the coupled microscopic cell problem is fully nonlinear. The strategy of the proof, namely two encapsulated fixed point arguments, motivated the formulation of an iterative procedure, its convergence is proven.
An interesting point for future work is the implementation of a numerical algorithm in order to compute a solution of the two scale model. A quantitative comparison of these numerical simulations to experiments in order to validate the model would be desirable.
Another goal for further investigations is the rigorous justification of the, up to now formal, derivation of the two scale model by asymptotic expansions. For the model without elasticity, this could be done, but it is not possible to apply the same methods to the model with elasticity, due to its much more complex structure.
Concerning the modeling, the description of the elastic effects could probably be done in a more realistic way. In particular, misfit between substrate and layer is in fact an interaction in both directions. This would lead to another elastic problem in the substrate with possibly another free boundary.
From the mathematical point of view, it would be interesting to study the methods of section 3.3, the macroscopic problem, in a more abstract setting. Evolution problems, where the corresponding stationary problem has limited regularity properties are rarely considered in the literature, and the ideas of the paper look quite promising to us.

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