

# **A Two Scale Model for Liquid Phase Epitaxy with Elasticity**

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## Abstract

Epitaxy, a special form of crystal growth, is a technically relevant process for the production of thin films and layers. It gives the possibility to 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 is the so-called liquid phase epitaxy. Thereby, single particles are deposited out of a supersaturated liquid solution on a substrate where they contribute to the growth process.

The thesis studies a two scale model including elasticity, introduced 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 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 a basis for an numerical algorithm.



## Zusammenfassung

Epitaxie ist ein technischer Kristallwachstumsprozess zur Herstellung dünner Kristallschichten. Diese weisen dabei oft Mikrostrukturen verschiedener Form und Ausprägung auf, wie zum Beispiel Stufen, Spiralen oder Pyramiden. Die Ausbildung dieser Mikrostrukturen wird unter anderem durch elastische Effekte in der epitaktischen Schicht beeinflusst. Es gibt verschiedene Varianten der Epitaxie, eine davon ist die sogenannte Flüssigphasenepitaxie. Dabei lagern sich einzelne Teilchen aus einer übersättigten flüssigen Lösung auf einem Substrat ab und tragen dort zum Wachstum bei. In dieser Arbeit wird ein Zweiskalenmodell zur Flüssigphasenepitaxie unter Berücksichtigung elastischer Verformungen untersucht. Dieses Modell wurde in [Ch. Eck, H. Emmerich. Liquid-phase epitaxy with elasticity. *Preprint 197*, DFG SPP 1095, 2006] eingeführt. Es besteht aus makroskopischen Navier-Stokes-Gleichungen und einer makroskopischen Konvektions-Diffusions-Gleichung für den Massentransport in der Flüssigkeit, sowie einem mikroskopischen Problem, zusammengesetzt aus einer Phasenfeldapproximation eines Burton-Cabrera-Frank-Modells zur Beschreibung der epitaktischen Schicht, einem Stokes System in der Flüssigkeit nahe der Schicht und einer Elastizitätsgleichung für die elastischen Effekte in der Schicht. Die einzelnen Teilprobleme sind durch geeignete Bedingungen gekoppelt.

Das Hauptresultat der Arbeit ist der Beweis der Existenz und Eindeutigkeit einer Lösung des Zweiskalenmodells mit Hilfe von Fixpunktargumenten. Des Weiteren wird eine iterative Lösungsstrategie vorgeschlagen, die auf der einen Seite die Beweisstruktur des Hauptresultats widerspiegelt, und auf der anderen Seite die Grundlage für einen numerischen Lösungsalgorithmus sein kann.



## Acknowledgement

I would like to remember Prof. Dr. Christof Eck, who passed away far too early in 2011. It was him who provided me the opportunity to work on that topic. The thesis is about his model and his project. Even if he could not see the final results of my work, he influenced many proofs and arguments by his support, especially that which are published in [21]. I hold him in grateful memory.

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*Michael Kutter*



# 1 Introduction

Many components of electronic devices, think for example of microchips, consist of multiple very thin layers, with thickness of several molecule or atom diameters. It is not possible to obtain such thin films by polishing, so other techniques have to be applied, such as controlled crystal growth. Epitaxy is a special form of crystal growth, where single particles (for example of silicon or a silicon-germanium alloy  $\text{Ge}_x\text{Si}_{1-x}$ ) are deposited on a substrate (made for example of silicon), where they can move on its surface, driven by diffusion, until they leave it again or until they contribute to a growing epitaxial layer. The layer thereby forms monomolecular steps, see Figure 1. In the case of the same material composition in substrate and layer the process is called homoepitaxy, else heteroepitaxy.

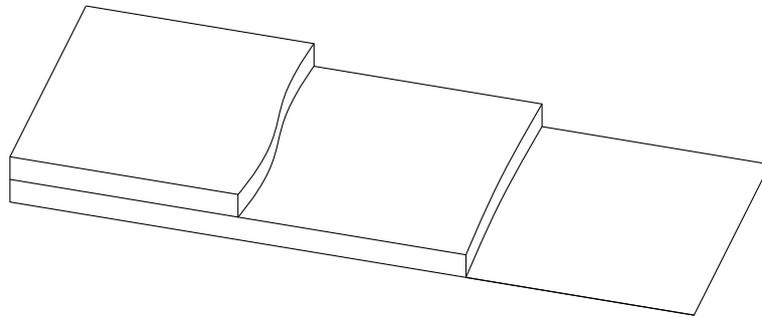


Figure 1: Schematic Visualization of a Stepped Epitaxial Layer.

Epitaxy is not the name of one process, but a broader term of several epitaxial techniques. Among others, there are molecular beam epitaxy (MBE) and liquid phase epitaxy (LPE), which are frequently used in technical applications. The main difference between these concerns the way of depositing the particles on the growing layer. In MBE, the particles are sent from effusion cells as molecular beams through high vacuum to the substrate, while in LPE they are transported through a supersaturated liquid solution by convection and diffusion.

The main application of epitaxial techniques lies in the production of semiconductor devices like solar cells, integrated circuits, lasers and light emitting diodes. During the growth process, the epitaxial layers usually generate microstructures of different morphologies such as steps, islands, spirals or pyramids, see Figure 2. These microstructures influence the physical properties of the layer, as for example the electric conductivity, and therefore, it is important to understand how they develop. Different aspects are important thereby, [13], [23], [51], and especially in the case of heteroepitaxy, elastic effects play a significant role. These effects are induced by a so-called misfit between substrate and layer, which occurs due to different crystal structures of the materials of the substrate and the layer.

In this thesis, a model for LPE is investigated, where elastic effects are included.

**Liquid Phase Epitaxy.** For a detailed description of the physical principles and the applications of LPE, see [6], [50]. The first model for epitaxial growth goes back to Burton, Cabrera and Frank (BCF model), [8]. It is a semi-discrete model: The diffusion process along the surface is described by continuum equations, while in perpendicular direction, the monomolecular steps are resolved in a discrete way. Originally, the model was developed to describe MBE, but almost all models for LPE base on it, too.

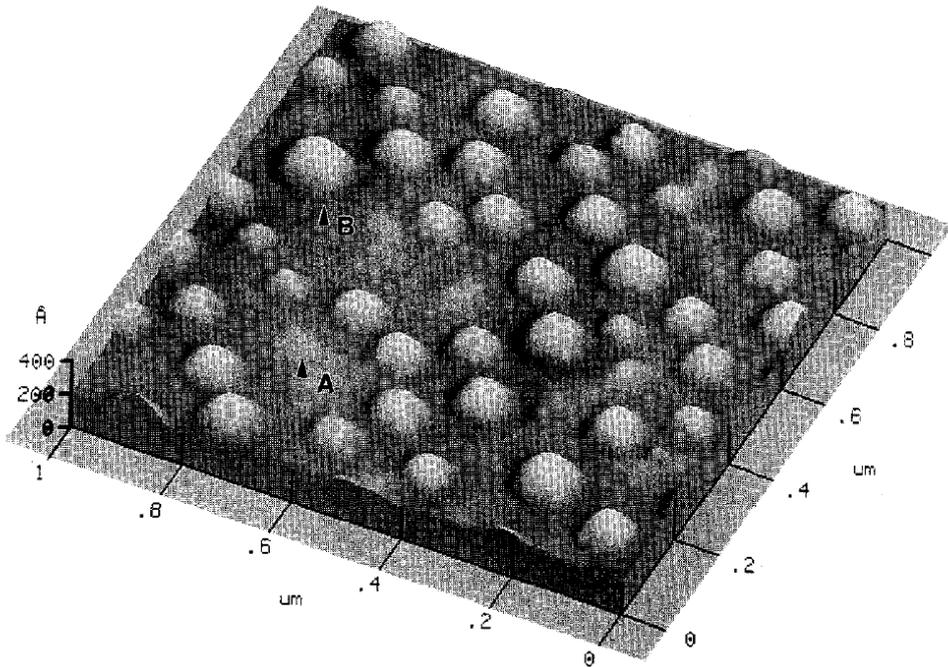


Figure 2: Experimentally observed Pyramidal Microstructure in  $\text{Ge}_{0.85}\text{Si}_{0.15}$  Growth on  $\text{Si}(001)$  from Bi Solution, see [13].

Besides the semi-discrete approach of Burton, Cabrera and Frank, other models have been developed in both directions: On the one hand, there are descriptions of the epitaxial growth process by purely continuum models, [37], [54], [56]. These models describe the height of the solid film by nonlinear partial differential equations and do not resolve the stepped structure of the surface. On the other hand, purely discrete models describe the movement of each particle and their interactions by kinetic Monte Carlo methods, [44]. The major disadvantage of these models is, that they are only applicable at very small length scales.

As a version of the BCF model, phase field models have been established, [17], [31], [36], [40]. Based on the ideas of diffuse interface models for phase transitions in solidification processes, see [9], the steps from one monomolecular layer to another are smoothed, where the thickness of the smooth transition region is controlled by a 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.

There are also hybrid models, such as that proposed in [33], where the nucleation of new monomolecular layers is modeled by kinetic Monte Carlo methods, but else, a phase field version of the BCF model is used.

Elastic effects have been considered in a purely continuum model, [56], in a purely discrete model, [44], and in a BCF model, [23].

Some models also include the so-called Ehrlich-Schwoebel barrier, [22], [46], [47]: It describes, that a particle is not as likely to be incorporated, if it approaches a step from above, as if it comes from below. This asymmetry induces an uphill current, see [37]. In [5] and [36], it is explained, how to include that in the BCF context.

In LPE in contrast to MBE, where the deposition of particles is usually modeled by a known deposition rate, a model for the volumic transport of particles in the liquid solution has to be coupled to the model for epitaxial growth. Thereby, not only diffusion but also convection should be included as pointed out in [32].

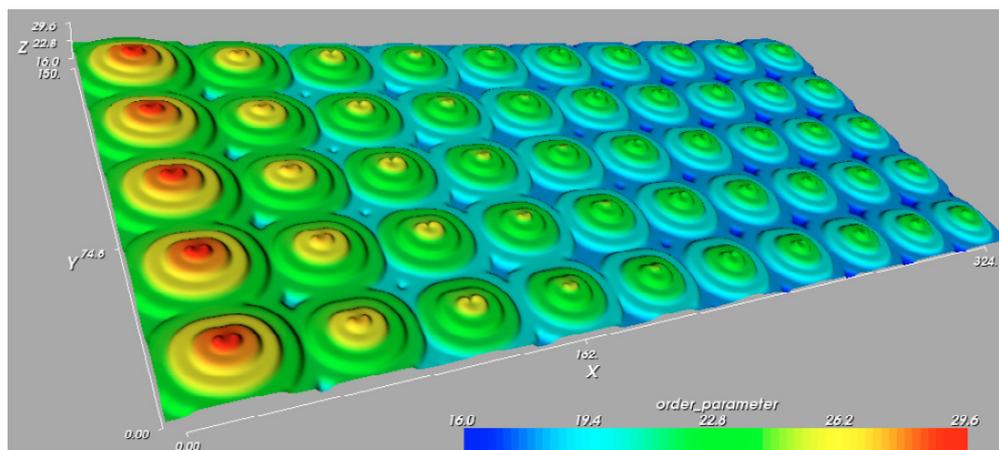


Figure 3: Simulation of an Epitaxial Layer using a Phase-Field-BCF Model, see [10].

Each of the three types of models (continuum, semi-discrete, discrete) has its advantages. Concerning the simulation, kinetic Monte-Carlo models are not able to compute epitaxy on large length scales, while purely continuum models do not fully resolve the microstructure. BCF type models, where phase field approximations suit better for this purpose, are a compromise between both, but nevertheless, the microstructure has to be resolved by a numerical grid, which makes the simulation of a technically relevant device almost impossible. New possibilities for an efficient implementation are opened up by the application of homogenization techniques, which leads to a formulation of two scale models.

**Homogenization in LPE.** Homogenization, [11], has proven to be a very powerful tool for example in the description of fluid flow in porous media, where in a simple case, Stokes equations have to be solved in a domain with unknown microstructures, [30]. Thereby, the inhomogeneous domain is replaced by a fictive homogeneous one, which possesses approximately the same macroscopic properties. In principle, homogenization methods can also be applied for problems, where the unknown microstructure is of interest and should be computed, see for example [14], [15], [16]. In these cases, it results in a so-called two or multi scale model, consisting of macroscopic equations (with homogenized domains, parameters, et cetera) which are coupled to microscopic cell problems for the determination of the microstructure. Usually, there is one cell problem in each macroscopic point.

For LPE, a two scale model has been derived in [17]. 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 [17].

The model of [17] was further developed in [18] and [19], where elastic effects are included. The main difference to [17] 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.

**Objective of the thesis.** The goal of the thesis is to analyze the two scale model with elasticity developed in [19]. The focus hereby lies on the proof of existence and uniqueness of a solution, but furthermore, a basis for the numerical treatment is laid. The model consists of macroscopic Navier-Stokes equations and a macroscopic convection-diffusion equation for the transport process in the liquid solution "far away" from the interface between liquid solution and solid layer, and of microscopic cell problems for processes near the interface. These are modeled by Stokes equations for the fluid flow, a linear elastic equation for the deformation in the solid layer and a phase field version of a BCF model for the evolution of the epitaxial surface.

**Outline.** In *chapter 2*, the notation is explained. Definitions are given, which are needed throughout the thesis, especially that of some important function spaces. Furthermore, several functional analytical tools are collected from literature which are frequently used in the proofs, and some results are adapted to the cases of the thesis.

*Chapter 3* presents and explains the model, starting from the non-homogenized physical

model. The original BCF version with sharp steps is explained as well as its phase field approximation. The ansatz for the derivation of the two scale model is given, and the model problem is stated precisely. The chapter concludes with a short discussion of the model.

*Chapter 4* proposes an iterative solving procedure with two objectives: On the one hand, it outlines a strategy how existence and uniqueness of a solution of the model can be proven via fixed point arguments, and on the other hand, it is a basis for an algorithm to solve the model problem numerically. The iteration consists of two encapsulated iterations, an inner for the microscopic cell problems and an outer for the coupling between the microscopic and the macroscopic problems. Convergence of the iterative procedure is proven.

The main chapter of the thesis is *chapter 5*, and it starts by stating the main result in section 5.1: The existence and uniqueness of a solution of the two scale model in suitable function spaces, under appropriate assumptions on the given data. Its proof is given in the following sections. First, the microscopic cell problem is investigated in section 5.2, where the macroscopic coupling data is supposed to be given. Thereto, the single microscopic problems, namely the Stokes problem, the elastic problem and the BCF problem are studied separately in sections 5.2.1 – 5.2.3, and their coupling is investigated in section 5.2.4. Existence and uniqueness of solutions of the coupled microscopic cell problems is proven using Banach's Fixed Point Theorem. Conversely, solvability of the macroscopic problem is shown in section 5.3 with the microscopic coupling data considered as given. Only the convection- diffusion problem is discussed since the Navier-Stokes equations decouple from the rest of the model. As last step in the proof of the main result, section 5.4 treats the coupling between the microscopic and the macroscopic parts, again by using Banach's Fixed Point Theorem.

Finally, *chapter 6* concludes with a short discussion of results and open problems.

Parts of this thesis are to find in [20] and [21] and another publication is in preparation.



## 2 Notation and some Basics

This chapter is devoted to some mathematical fundamentals of this thesis. On the one hand, definitions are provided especially that of several function spaces. On the other hand, some results are given, which are frequently used in chapter 5, such as embedding theorems, basic inequalities, Banach's Fixed Point Theorem, et cetera. Few of them are not to find in common literature and, in these cases, proofs are presented. The rest is supplied by references.

### 2.1 Basic Notation

In  $\mathbb{R}^n$ , the  $i$ -th standard coordinate vector is denoted by  $e_i$ . For  $x = (x_1, \dots, x_n)^\top \in \mathbb{R}^n$ ,  $|x|$  is the Euclidean norm of  $x$ . If  $\Omega \subset \mathbb{R}^n$ , then  $\partial\Omega$  is its boundary,  $\overline{\Omega}$  its closure and  $|\Omega|$  its volume.

The scalar product between two vectors  $x$  and  $y$  in  $\mathbb{R}^n$  is denoted by  $x \cdot y$ , the scalar product between two matrices  $A = (a_{ij})$  and  $B = (b_{ij})$ ,  $i = 1, \dots, n$ ,  $j = 1, \dots, m$ , in  $\mathbb{R}^{n \times m}$  by

$$A : B = \sum_{\substack{i=1, \dots, n \\ j=1, \dots, m}} a_{ij} b_{ij}.$$

Consider a time interval  $I = [0, T]$  and a domain  $\Omega \subset \mathbb{R}^n$ . For a function  $f : I \times \Omega \rightarrow \mathbb{R}$ , the partial derivatives with respect to the time variable  $t$  or the space variable  $x_i$  are denoted by  $\partial_t f$  or  $\partial_{x_i} f$  respectively. If  $\beta = (\beta_1, \dots, \beta_n) \in \mathbb{N}_0^n$  is a multi-index with  $|\beta| = \beta_1 + \dots + \beta_n$ , then the spatial derivatives are expressed by

$$D^\beta f := \partial_{x_1}^{\beta_1} \dots \partial_{x_n}^{\beta_n} f, \quad D^k f := \{D^\beta f \mid |\beta| = k\} \quad \text{and} \quad |D^k f| := \left( \sum_{|\beta|=k} |D^\beta f|^2 \right)^{\frac{1}{2}}.$$

For vector valued functions  $f : I \times \Omega \rightarrow \mathbb{R}^m$ ,  $f = (f_1, \dots, f_m)$ , it is  $D^\beta f := (D^\beta f_1, \dots, D^\beta f_m)$  et cetera.

In the special case of first order derivatives, the gradient of  $f$  is defined by

$$\nabla f := \begin{pmatrix} \partial_{x_1} f_1 & \cdots & \partial_{x_1} f_m \\ \vdots & \ddots & \vdots \\ \partial_{x_n} f_1 & \cdots & \partial_{x_n} f_m \end{pmatrix},$$

and, in the case  $n = m$ , its symmetric part by

$$e(f) := \frac{1}{2} (\nabla f + (\nabla f)^\top).$$

If there is the possibility of confusion, because of the occurrence of different spatial variables  $x \in \mathbb{R}^n$  and  $y \in \mathbb{R}^n$ , the corresponding derivatives are supplied with a respective index such as  $\nabla_x f$ ,  $\nabla_y f$ ,  $e_x(f)$ , et cetera.

## 2.2 Hölder Spaces

Denote by  $C^\infty(\Omega)$  the space of infinitely differentiable functions, defined in a domain  $\Omega \subset \mathbb{R}^n$ . For  $k \in \mathbb{N}_0$ , let  $C^k(\Omega)$  be the space of  $k$ -times differentiable functions, which have bounded norm

$$\|f\|_{C^k(\Omega)} = \sum_{|\beta| \leq k} \sup_{x \in \Omega} |D^\beta f(x)|.$$

$C_0^k(\Omega)$  denotes the subset of  $C^k(\Omega)$  of functions with compact support in  $\Omega$ . For  $k \in \mathbb{N}_0$  and  $0 < \alpha \leq 1$ , it is

$$C^{k+\alpha}(\Omega) := \{f \in C^k(\Omega) \mid D^k f \in C^\alpha(\Omega)\}$$

the classical Hölder space, equipped with the norm

$$\|f\|_{C^{k+\alpha}(\Omega)} = \|f\|_{C^k(\Omega)} + \max_{|\beta|=k} \sup_{x \neq y \in \Omega} \frac{|D^\beta f(x) - D^\beta f(y)|}{|x - y|^\alpha}.$$

Sometimes, the more compact notation  $C^\theta(\Omega)$  with  $\theta = k + \alpha \in \mathbb{R}_0^+$  is used.

In the context of evolution equations, for example parabolic partial differential equations, functions with different regularity properties with respect to time and space are of particular importance.

**Definition 2.1** (Some Hölder spaces with anisotropic regularity in time and space). *Let be  $k, \ell \in \mathbb{N}_0$ ,  $0 \leq \alpha, \alpha_1, \alpha_2 \leq 1$ ,  $I = [0, T]$  and  $\Omega \subset \mathbb{R}^n$ .*

$$\begin{aligned} C^{0,k+\alpha}(I \times \Omega) &= \{f \in C(I \times \Omega) \mid f(t, \cdot) \in C^{k+\alpha}(\Omega), \forall t \in I\}, \\ C^{k+\alpha,0}(I \times \Omega) &= \{f \in C(I \times \Omega) \mid f(\cdot, x) \in C^{k+\alpha}(I), \forall x \in \Omega\}, \\ C^{\alpha_1, \alpha_2}(I \times \Omega) &= C^{\alpha_1, 0}(I \times \Omega) \cap C^{0, \alpha_2}(I \times \Omega), \\ C^{k, \ell}(I \times \Omega) &= C^{k, 0}(I \times \Omega) \cap C^{0, \ell}(I \times \Omega), \\ C^{k+\alpha_1, \ell+\alpha_2}(I \times \Omega) &= \{f \in C^{k, \ell}(I \times \Omega) \mid \partial_t^m f, D^\beta f \in C^{\alpha_1, \alpha_2}(I \times \Omega), m \leq k, |\beta| \leq \ell\}. \end{aligned}$$

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

## 2.3 Lebesgue and Sobolev spaces

For  $1 \leq r \leq \infty$ ,  $L_r(\Omega)$  denotes the Lebesgue space of functions whose  $r$ -th power is integrable ( $r < \infty$ ) or which are essentially bounded ( $r = \infty$ ), equipped with the norm

$$\|f\|_{L_r(\Omega)} = \begin{cases} \left( \int_{\Omega} |f|^r dx \right)^{\frac{1}{r}}, & r < \infty, \\ \text{esssup}_{x \in \Omega} |f(x)|, & r = \infty. \end{cases}$$

For  $k \in \mathbb{N}_0$  and  $1 \leq r \leq \infty$ , it is  $W_r^k(\Omega)$  the Sobolev space of functions whose derivatives up to order  $k$  belong to  $L_r(\Omega)$ , equipped with the norm

$$\|f\|_{W_r^k(\Omega)} = \begin{cases} \left( \sum_{|\beta| \leq k} \|D^\beta f\|_{L_r(\Omega)}^r \right)^{\frac{1}{r}}, & r < \infty, \\ \sum_{|\beta| \leq k} \|D^\beta f\|_{L_\infty(\Omega)}, & r = \infty. \end{cases}$$

Additionally, if  $0 < \alpha < 1$  and  $s = k + \alpha$ ,  $W_r^s(\Omega)$  is the Sobolev-Slobodeckij space, equipped with the norm

$$\|f\|_{W_r^s(\Omega)} = \left( \|f\|_{W_r^k(\Omega)}^r + \sum_{|\beta|=k} \int_{\Omega} \int_{\Omega} \frac{|D^\beta f(x) - D^\beta f(y)|^r}{|x - y|^{n+\alpha r}} dx dy \right)^{\frac{1}{r}}.$$

The Hilbert spaces  $W_2^s(\Omega)$  are denoted by  $H^s(\Omega)$ .  $W_r^s(\Omega)'$  and  $H^s(\Omega)'$  denote the dual spaces of  $W_r^s(\Omega)$  and  $H^s(\Omega)$ , respectively.

The anisotropic Sobolev spaces  $W_r^{s_1, s_2}(I \times \Omega)$  are defined analogously to the anisotropic Hölder spaces in Definition 2.1.

Functions in  $W_r^s(\Omega)$  are only defined almost everywhere in  $\Omega$ . Since the boundary  $\partial\Omega$  usually is a set of measure zero (with respect to the  $n$ -dimensional Lebesgue measure), boundary values of a function  $f \in W_r^s(\Omega)$  are not well-defined in the classical sense. Therefore, the notion of traces is introduced, see for example [27], chapter 1.5, Theorem 1.5.1.2:

**Theorem 2.2** (Traces). *Let  $\Omega$  be a bounded open subset of  $\mathbb{R}^n$  with a  $C^{k+1}$  boundary  $\partial\Omega$ ,  $k$  an integer  $\geq 0$ . Assume  $s - \frac{1}{r}$  is not an integer,  $s \leq k + 1$ ,  $s - \frac{1}{r} = \ell + \sigma$ ,  $0 < \sigma < 1$ ,  $\ell$  an integer  $\geq 0$  and  $n$  the outer normal vector. Then the trace operator*

$$\text{tr}: f \mapsto \left( f, \frac{\partial f}{\partial n}, \dots, \frac{\partial^\ell f}{\partial n^\ell} \right) \Big|_{\partial\Omega}$$

which is defined for  $f \in C^{k+1}(\overline{\Omega})$ , has a unique continuous extension as an operator from

$$W_r^s(\Omega) \quad \text{onto} \quad \prod_{j=0}^{\ell} W_r^{s-j-\frac{1}{r}}(\partial\Omega).$$

This operator has a right continuous inverse which does not depend on  $r$ .

The space  $\dot{W}_r^s(\Omega)$  is the subspace of  $W_r^s(\Omega)$  of functions, which trace on  $\partial\Omega$  is zero. In the case of an unbounded domain  $\Omega$ , the subscript loc in  $W_{r, \text{loc}}^1(\Omega)$  denotes the set of functions, which belong to  $W_r^1(\tilde{\Omega})$  for any bounded  $\tilde{\Omega} \subset \Omega$  with Lipschitz boundary  $\partial\tilde{\Omega}$ .

Finally, here are some density properties of Sobolev spaces:

**Theorem 2.3.** *Suppose that  $k \in \mathbb{N}_0$ ,  $1 \leq r < \infty$  and that  $\Omega$  is a bounded domain with Lipschitz boundary. Then  $C^\infty(\Omega)$  is dense in  $W_r^k(\Omega)$ .*

*If  $\Omega$  has Lipschitz boundary, but is not bounded, then the set of restrictions to  $\Omega$  of functions in  $C_0^\infty(\mathbb{R}^n)$  is dense in  $W_r^k(\Omega)$ .*

For the proof, see [1], Theorem 3.17, p.67, and Theorem 3.22, pp.68-70. An obvious consequence is the following lemma:

**Lemma 2.4.** *Suppose  $k \in \mathbb{N}_0$ ,  $1 \leq r < \infty$ .  $W_r^k(\Omega)$  is dense in  $L_r(\Omega)$ .*

There are also the following density properties of the dual spaces, see [1], 3.14, p.65:

**Theorem 2.5.** *Suppose  $k \in \mathbb{N}_0$ ,  $1 < r < \infty$  and  $\frac{1}{r} + \frac{1}{r'} = 1$ .  $L_r(\Omega)$  is dense in  $(W_r^k(\Omega))'$ .*

**Lemma 2.6.** *Suppose  $k \in \mathbb{N}_0$ ,  $1 < r < \infty$  and  $\frac{1}{r} + \frac{1}{r'} = 1$ .  $W_r^k(\Omega)$  is dense in  $(W_r^k(\Omega))'$ .*

*Proof.* Suppose  $F \in (W_r^k(\Omega))'$ . Since  $L_r(\Omega)$  is dense in  $(W_r^k(\Omega))'$ , see Theorem 2.5, there is a sequence  $(F_n)_{n \in \mathbb{N}} \subset L_r(\Omega)$  with

$$\|F_n - F\|_{(W_r^k(\Omega))'} \rightarrow 0, \quad \text{for } n \rightarrow \infty.$$

Since  $W_r^k(\Omega)$  is dense in  $L_r(\Omega)$ , see Lemma 2.4, there is for each  $n \in \mathbb{N}$  a sequence  $(f_{nk})_{k \in \mathbb{N}} \subset W_r^k(\Omega)$  with

$$\|F_n - f_{nk}\|_{L_r(\Omega)} \rightarrow 0, \quad \text{for } k \rightarrow \infty.$$

It follows that

$$\|F - f_{nk}\|_{(W_r^k(\Omega))'} \leq \|F - F_n\|_{(W_r^k(\Omega))'} + \|F_n - f_{nk}\|_{(W_r^k(\Omega))'},$$

and due to Hölder's inequality

$$\|F_n - f_{nk}\|_{(W_r^k(\Omega))'} = \sup_{\substack{w \in W_r^1(\Omega), \\ \|w\|_{W_r^1(\Omega)} = 1}} \int_{\Omega} (F_n - f_{nk})w \, dx \leq \|F_n - f_{nk}\|_{L_r(\Omega)}.$$

For any  $\varepsilon > 0$  and any  $n \in \mathbb{N}$ , there is a number  $K_n \in \mathbb{N}$  such that

$$\|F_n - f_{nk}\|_{L_r(\Omega)} < \frac{\varepsilon}{2}, \quad \text{for all } k \geq K_n.$$

Furthermore, there is  $N \in \mathbb{N}$  such that

$$\|F_n - F\|_{(W_r^k(\Omega))'} \leq \frac{\varepsilon}{2}, \quad \text{for all } n \geq N,$$

and consequently

$$\|F - f_{nK_n}\|_{(W_r^k(\Omega))'} \leq \|F - F_n\|_{(W_r^k(\Omega))'} + \|F_n - f_{nK_n}\|_{L_r(\Omega)} < \varepsilon, \quad \text{for all } n \geq N.$$

□

## 2.4 Periodicity

Periodic functions play an important role in this thesis. Therefore, the notion of periodicity is stated precisely, see also [11], [17]:

**Definition 2.7** ( $Y$ -periodicity). *An open, bounded and simply connected domain  $Y \subset \mathbb{R}^n$  with Lipschitz boundary is called **periodicity cell**, if  $\mathbb{R}^n$  can be represented as a union of shifted copies of  $Y$  with empty intersection:*

$$\mathbb{R}^n = \bigcup_{z \in M_Y} (z + \bar{Y}), \quad (z_1 + Y) \cap (z_2 + Y) = \emptyset \quad \text{for } z_1 \neq z_2 \in M_Y,$$

where  $M_Y \subset \mathbb{R}^n$  is a countable set of shifts. A function  $f$  defined a.e. in  $\mathbb{R}^n$  is called  $Y$ -periodic if

$$f(z_1 + y) = f(z_2 + y) \quad \text{for almost all } y \in Y \quad \text{and all } z_1, z_2 \in M_Y.$$

The simplest example for a periodicity cell is  $Y = [(0, 1)]^n$  and  $M_Y = \mathbb{Z}^n$ .

**Definition 2.8** (Spaces of  $Y$ -periodic functions). *Suppose  $Y$  is a periodicity cell.*

- i) *For  $k \in \mathbb{N}_0$  and  $0 \leq \alpha \leq 1$ , the space  $C_{\text{per}}^{k+\alpha}(Y)$  is the subspace of  $C^{k+\alpha}(\mathbb{R}^n)$  of  $Y$ -periodic functions. The space  $C_{\text{per}}^\infty(Y)$  is the subspace of  $C^\infty(\mathbb{R}^n)$  of  $Y$ -periodic functions.*
- ii) *The space  $W_{r,\text{per}}^s(Y)$  with  $s \in \mathbb{R}_0^+$  and  $1 \leq r \leq \infty$  is the closure of  $C_{\text{per}}^\infty(Y)$  with respect to the  $W_r^s(Y)$ -norm.*

In chapter 5, there occur microscopic domains, which have the form  $Y \times \mathbb{R} \subset \mathbb{R}^3$  (or are subdomains thereof). The following notation is used:

Let be  $X(Y \times \mathbb{R}) \in \{C^{k+\alpha}(Y \times \mathbb{R}), W_r^k(Y \times \mathbb{R})\}$ , where  $k \in \mathbb{N}_0$ ,  $0 \leq \alpha < 1$ ,  $1 \leq r \leq \infty$ . Then denote by  $X_{\text{per}}(Y \times \mathbb{R}) \subset X(Y \times \mathbb{R})$  the subspace of functions, which are  $Y$ -periodic in  $X(Q_l)$  with respect to  $y_1$  and  $y_2$  in the sense of definition 2.8. There is no periodicity assumption concerning  $y_3$ .

For anisotropic spaces as e.g.  $C_{\text{per}}^{1,2+\alpha}(I \times Y)$ , the lower index "per" indicates the corresponding subspace which consists of  $Y$ -periodic functions.

## 2.5 Basic Inequalities

### Young's Inequality

Suppose  $a, b > 0$ ,  $1 < r, r' < \infty$  and  $\frac{1}{r} + \frac{1}{r'} = 1$ . Then

$$ab \leq \frac{a^r}{r} + \frac{b^{r'}}{r'}. \quad (2.1)$$

Furthermore, if  $\varepsilon > 0$ , then

$$ab \leq \varepsilon a^r + c(\varepsilon) b^{r'}, \quad (2.2)$$

with  $c(\varepsilon) = \frac{1}{(\varepsilon r)^{r'/r}}$ . For the proof, see e.g. [25], p.622.

### Hölder's Inequality

Suppose  $1 \leq r, r' \leq \infty$  and  $\frac{1}{r} + \frac{1}{r'} = 1$ . Then for  $f \in L_r(\Omega)$  and  $g \in L_{r'}(\Omega)$ , it is

$$\int_{\Omega} |fg| dx \leq \left( \int_{\Omega} |f|^r dx \right)^{\frac{1}{r}} \left( \int_{\Omega} |g|^{r'} dx \right)^{\frac{1}{r'}}. \quad (2.3)$$

For the proof, see e.g. [25], p.623.

### Gronwall's Inequality

Let  $f(t)$  be a nonnegative integrable function on  $I = [0, T]$  which satisfies for a.a.  $t \in I$

$$f(t) \leq c_1 \int_0^t f(s) ds + c_2$$

with constants  $c_1, c_2 \geq 0$ . Then

$$f(t) \leq c_2 (1 + c_1 t e^{c_1 t}) \quad (2.4)$$

for a.a.  $t \in I$ . In particular,  $f(t) \equiv 0$  a.e. in  $I$ , if  $c_2 = 0$ . For the proof, see e.g. [25], p.625.

### Poincaré's Inequality

Suppose  $\Omega = [0, d] \times \mathbb{R}^{n-1}$  with  $d > 0$ , then there exists a constant  $k$ , which is proportional to  $d$ , such that

$$\|f\|_{L_r(\Omega)} \leq k \|\nabla f\|_{L_r(\Omega)}, \quad (2.5)$$

for all  $f \in W_r^1(\Omega)$  with  $f|_{x_1=0} = 0$ . This can be proven as Theorem 6.30 in [1], pp.183-184.

## 2.6 Embeddings and Interpolation

The proofs of section 5.2 use embedding and interpolation theorems several times. Some important ones are stated here.

The following result about the famous Sobolev embeddings can be found e.g. in [27], Ch.1.4.4, pp.27-28.

**Theorem 2.9** (Embedding theorem). *Suppose  $\Omega$  has a Lipschitz boundary and  $s_1 \in \mathbb{R}_0^+$ ,  $s_2 \in \mathbb{R}$  with  $s_1 \geq s_2$ , and  $1 < r_1, r_2 < \infty$  such that  $s_1 - \frac{n}{r_1} = s_2 - \frac{n}{r_2}$ . Then the embedding*

$$W_{r_1}^{s_1}(\Omega) \hookrightarrow W_{r_2}^{s_2}(\Omega)$$

*exists and is continuous. If  $\Omega$  is bounded, the statement is true for  $s_1 - \frac{n}{r_1} \geq s_2 - \frac{n}{r_2}$ .*

If  $s \in \mathbb{R}^+$ ,  $1 \leq r \leq \infty$ ,  $k \in \mathbb{N}_0$  and  $0 < \alpha < 1$  such that  $s - \frac{n}{r}$  is not an integer and  $s - \frac{n}{r} = k + \alpha$ . Then the embedding

$$W_r^s(\Omega) \hookrightarrow C^{k+\alpha}(\bar{\Omega})$$

exists and is continuous. In the case that  $s - \frac{n}{r} = k$  is an integer, the continuous embedding

$$W_r^s(\Omega) \hookrightarrow C^{(k-1)+\alpha}(\bar{\Omega})$$

exists for any  $0 \leq \alpha < 1$ .

Next, some interpolatory inclusions in Hölder and Sobolev spaces are provided. They result from interpolation estimates, such as that of the following theorem:

**Theorem 2.10** (Interpolation estimate for intermediate Hölder spaces). *Suppose that  $\Omega$  has an uniform  $C^{\theta_2}$ -smooth boundary and that  $\theta_1, \theta_2, \theta \in \mathbb{R}_0^+$  with  $\theta_1 < \theta < \theta_2$ . Any function  $f \in C^{\theta_2}(\Omega)$  satisfies the estimate*

$$\|f\|_{C^\theta(\Omega)} \leq c \|f\|_{C^{\theta_1}(\Omega)}^{1-\lambda} \|f\|_{C^{\theta_2}(\Omega)}^\lambda,$$

with  $\lambda = \frac{\theta - \theta_1}{\theta_2 - \theta_1}$ .

This follows from [38], Proposition 1.1.3, p.13. For spaces with anisotropic regularity in time and space, a direct consequence of Thm. 2.10 is the following lemma, see [38], Prop. 1.1.4, p.13:

**Lemma 2.11.** *Suppose  $f \in C^{\alpha, 2\alpha}(I \times \Omega)$  and define the function  $\tilde{f}: t \mapsto \tilde{f}(t) := f(t, \cdot)$ . Then, for any  $0 \leq \beta \leq \alpha \leq \frac{1}{2}$ , it is  $\tilde{f} \in C^{\alpha-\beta}(I, C^{2\beta}(\Omega))$  and satisfies*

$$\|\tilde{f}\|_{C^{\alpha-\beta}(I, C^{2\beta}(\Omega))} \leq c \|f\|_{C^{\alpha, 2\alpha}(I \times \Omega)}.$$

$f$  and  $\tilde{f}$  in Lemma 2.11 are basically the same functions, only considered from different point of views:

- $f$  is considered as a function depending on  $x$  and  $t$  with values in  $\mathbb{R}$  or  $\mathbb{R}^n$ .
- $\tilde{f}$  only depends on  $t$ , but has values in a function space  $X$ , that consists of functions  $\Omega \rightarrow \mathbb{R}$  or  $\Omega \rightarrow \mathbb{R}^n$ , i.e.  $\tilde{f}: I \rightarrow X$ . In the previous Lemma it is  $X = C^{2\beta}(\Omega)$ .

Casually speaking, it is " $f = \tilde{f}$ " even if this is formally not correct. In the same sloppy manner, Lemma 2.11 states: " $C^{\alpha, 2\alpha}(I \times \Omega) \hookrightarrow C^{\alpha-\beta}(I, C^{2\beta}(\Omega))$  with continuous embedding". From here on, this thesis will not distinguish between  $f$  and  $\tilde{f}$  any more in order to simplify the notation.

Another example for interpolation between time and space regularity is the following, see [38], Lemma 5.1.1, p.176:

**Lemma 2.12.** *Suppose  $0 \leq \alpha \leq \frac{1}{2}$ . The embedding*

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

*exists and is continuous.*

In Sobolev spaces an analogous result as that of Theorem 2.10 is:

**Theorem 2.13** (Interpolation estimate for intermediate Sobolev spaces). *Suppose that  $\Omega$  is bounded with  $C^{k_1}$ -smooth boundary and that  $1 < r_1, r_2 < \infty$ ,  $k_1 \geq k_2 \geq 0$ ,  $0 < \lambda < 1$  and  $k := \lambda k_1 + (1 - \lambda)k_2$ ,  $\frac{1}{r} := \frac{\lambda}{r_1} + \frac{1-\lambda}{r_2}$ . Any function  $f \in W_{r_1}^{k_1}(\Omega) \cap W_{r_2}^{k_2}(\Omega)$  belongs to  $W_r^k(\Omega)$  and satisfies the estimate*

$$\|f\|_{W_r^k(\Omega)} \leq c \|f\|_{W_{r_1}^{k_1}(\Omega)}^\lambda \|f\|_{W_{r_2}^{k_2}(\Omega)}^{1-\lambda}.$$

This follows from [7], Theorem 6.4.5, pp.152-153, see also [14], Theorem 2.2.4, p.23. A consequence for spaces with anisotropic regularity in time and space in this case is Corollary 2.2.6 in [14], p.23. It states:

**Lemma 2.14.** *Suppose that  $I = [0, T]$  and  $\Omega$  is bounded with  $C^k$ -smooth boundary. Then for  $0 < r < \infty$ ,  $k, \ell \geq 0$  and  $0 < \lambda < 1$ , every function  $f \in W_r^{\ell, k}(I \times \Omega)$  belongs to  $W_r^{\lambda \ell}(I, W_r^{k(1-\lambda)}(\Omega))$  and satisfies the estimate*

$$\|f\|_{W_r^{\lambda \ell}(I, W_r^{k(1-\lambda)}(\Omega))} \leq \|f\|_{W_r^{\ell, k}(I \times \Omega)}.$$

In chapter 5, an interpolatory inclusion is used where the dual space  $(W_r^1(\Omega))'$  is involved. A proof is given here:

**Proposition 2.15** (An interpolation estimate between  $W_r^1(\Omega)$  and  $(W_r^1(\Omega))'$ ). *Suppose  $2 \leq r < \infty$ ,  $\frac{1}{r} + \frac{1}{r'} = 1$  and  $f \in W_r^1(\Omega)$ . Then*

$$\|f\|_{L_r(\Omega)} \leq c \|f\|_{(W_r^1(\Omega))'}^{\frac{1}{r}} \|f\|_{W_r^1(\Omega)}^{1-\frac{1}{r}}.$$

*Proof.* Any  $f \in L_r(\Omega)$  induces an element of  $(W_r^1(\Omega))'$ , again denoted by  $f$ , by

$$\begin{aligned} \langle f, w \rangle &:= \int_{\Omega} f w \, dx, \quad \forall w \in W_r^1(\Omega), \\ \|f\|_{(W_r^1(\Omega))'} &= \sup_{\substack{w \in W_r^1(\Omega), \\ \|w\|_{W_r^1(\Omega)}=1}} \langle f, w \rangle. \end{aligned}$$

Note that, if  $f \in L_r(\Omega)$ , then  $|f|^{r-1} \in L_{r'}(\Omega)$  with

$$\|f|^{r-1}\|_{L_{r'}(\Omega)} = \left( \int_{\Omega} |f|^{(r-1)r'} \, dx \right)^{\frac{1}{r'}} = \left( \int_{\Omega} |f|^r \, dx \right)^{\frac{r-1}{r}} = \|f\|_{L_r(\Omega)}^{r-1}.$$

since  $(r-1)r' = r$  and  $\frac{1}{r'} = \frac{r-1}{r}$ . If  $f$  possesses weak derivatives  $\nabla f$ , then

$$\nabla|f| = \text{sign}(f)\nabla f, \quad \text{where} \quad \text{sign}(f)(x) = \begin{cases} 1, & f(x) > 0, \\ 0, & f(x) = 0, \\ -1 & f(x) < 0, \end{cases}$$

see [12], Satz 5.20, p.96. Furthermore, the weak derivatives of  $f|f|^{r-2}$  are due to the product rule

$$\nabla(f|f|^{r-2}) = |f|^{r-2}\nabla f + \text{sign}(f)(r-2)f|f|^{r-3}\nabla f,$$

and it follows with Young's inequality

$$|\nabla(f|f|^{r-2})| \leq c|f|^{r-2}|\nabla f| \leq c(|f|^{r-1} + |\nabla f|^{r-1}).$$

Therefore, if  $f \in W_r^1(\Omega)$ , then  $f|f|^{r-2} \in W_{r'}^1(\Omega)$  with

$$\|f|f|^{r-2}\|_{W_{r'}^1(\Omega)} \leq c\|f\|_{W_r^1(\Omega)}^{r-1}.$$

These preparations lead to

$$\begin{aligned} \|f\|_{L_r(\Omega)}^r &= \int_{\Omega} |f|^r dx \\ &= \int_{\Omega} f |f|^{r-2} dx \\ &= \|f|f|^{r-2}\|_{W_{r'}^1(\Omega)} \int_{\Omega} f \frac{|f|^{r-2}}{\|f|f|^{r-2}\|_{W_{r'}^1(\Omega)}} dx \\ &\leq \|f\|_{W_r^1(\Omega)}^{r-1} \|f\|_{(W_{r'}^1(\Omega))'} \end{aligned}$$

Taking the  $r$ -th root on both sides gives the result.  $\square$

**Lemma 2.16.** *Suppose  $2 \leq r < \infty$  and  $f \in C^1(I, (W_r^1(\Omega))') \cap C(I, W_r^1(\Omega))$ . Then  $f \in C^{\frac{1}{r}}(I, L_r(\Omega))$  with*

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

*Proof.* Proposition 2.15 and Young's inequality imply for  $t_1 \neq t_2 \in I$

$$\begin{aligned} \frac{\|f(t_1) - f(t_2)\|_{L_r(\Omega)}}{|t_1 - t_2|^{\frac{1}{r}}} &\leq c \left( \frac{\|f(t_1) - f(t_2)\|_{(W_r^1(\Omega))'}}{|t_1 - t_2|} \right)^{\frac{1}{r}} \|f(t_1) - f(t_2)\|_{W_r^1(\Omega)}^{1-\frac{1}{r}} \\ &\leq c \|f\|_{C^1(I, (W_r^1(\Omega))')}^{\frac{1}{r}} \|f\|_{C(I, W_r^1(\Omega))}^{1-\frac{1}{r}} \\ &\leq c \left( \|f\|_{C^1(I, (W_r^1(\Omega))')} + \|f\|_{C(I, W_r^1(\Omega))} \right). \end{aligned}$$

Moreover

$$\|f(t)\|_{L_r(\Omega)} \leq \|f(t)\|_{W_r^1(\Omega)}, \quad \forall t \in I,$$

and thus

$$\begin{aligned} \|f\|_{C^{\frac{1}{r}}(I, L_r(\Omega))} &= \max_{t \in I} \|f(t)\|_{L_r(\Omega)} + \sup_{t_1 \neq t_2 \in I} \frac{\|f(t_1) - f(t_2)\|_{L_r(\Omega)}}{|t_1 - t_2|^{\frac{1}{r}}} \\ &\leq c \left( \|f\|_{C^1(I, (W_r^1(\Omega))^r)} + \|f\|_{C(I, W_r^1(\Omega))} \right). \end{aligned}$$

□

## 2.7 Banach's Fixed Point and Lax-Milgram's Theorem

Both theorems are used frequently in chapter 5 and are therefore provided here:

**Theorem 2.17** (Lax-Milgram). *Suppose  $H$  is a real Hilbert space and*

$$a: H \times H \rightarrow \mathbb{R}$$

*a bilinear form that satisfies for all  $u, v \in H$*

$$a(u, v) \leq c_1 \|u\|_H \|v\|_H, \quad (\text{Continuity})$$

$$a(u, u) \geq c_2 \|u\|_H^2, \quad (H\text{-Ellipticity})$$

*with constants  $c_1, c_2 > 0$ . Then, for any element  $\ell$  of the dual space  $H'$ , there exists a unique element  $u \in H$  such that*

$$a(u, v) = \langle \ell, v \rangle, \quad \forall v \in H.$$

*Furthermore, there exists a constant  $c > 0$  such that*

$$\|u\|_H \leq c \|\ell\|_{H'}.$$

For a proof, see for example [43], Theorem 9.14, pp.290-292.

**Theorem 2.18** (Banach's Fixed Point Theorem). *Suppose  $M \subseteq X$  is a non-empty closed subset of a complete metric space  $(X, d)$  and  $T$  is an operator*

$$T: M \subset X \rightarrow M,$$

*which is a strict contraction, that means that there is a number  $0 \leq k < 1$  such that*

$$d(Tx, Ty) \leq kd(x, y), \quad \forall x, y \in M.$$

*Then,  $T$  has a unique fixed point  $x \in M$ . Furthermore, the sequence  $(x_n)_{n \in \mathbb{N}_0}$ , defined by*

$$x_0 \in M, \quad x_{n+1} := Tx_n, \quad n \in \mathbb{N}_0,$$

*converges to  $x$  for any  $x_0 \in M$ , and satisfies the a priori estimate*

$$d(x_n, x) \leq \frac{k^n}{1-k} d(x_0, x_1).$$

For a proof, see for example [57], Theorem 1.A, pp.17-18.

## 2.8 From the Theory of Semigroups

Some tools from semigroup-theory are used in section 5.3. In view of the proofs there, some basic terms are provided here. The following definitions coincide with the terminology in [38]. Further information can be found there, another textbook on that topic is for example [41].

Suppose  $X$  is a Banach space. The space of bounded linear functionals  $X \rightarrow X$  is denoted by  $L(X)$ . Consider a linear operator

$$A: D(A) \subset X \rightarrow X,$$

with domain  $D(A)$ . The **resolvent set**  $\rho(A)$  is defined by

$$\rho(A) := \{\lambda \in \mathbb{C} \mid (\lambda \mathbf{I} - A)^{-1} \text{ exists and belongs to } L(X)\}.$$

The **spectrum** of  $A$  is  $\varsigma(A) := \mathbb{C} \setminus \rho(A)$ . For  $\lambda \in \rho(A)$ , the operator

$$R(\lambda, A) := (\lambda \mathbf{I} - A)^{-1} : X \rightarrow X$$

is called **resolvent operator** or simply **resolvent**. The operator  $A$  is said to be **sectorial**, if there are constants  $\omega \in \mathbb{R}$ ,  $\frac{\pi}{2} < \theta < \pi$  and  $M > 0$  such that

$$(i) \quad \rho(A) \supset S_{\theta, \omega} := \{\lambda \in \mathbb{C} \mid \lambda \neq \omega, |\arg(\lambda - \omega)| < \theta\},$$

$$(ii) \quad \|R(\lambda, A)\|_{L(X)} \leq \frac{M}{|\lambda - \omega|}, \quad \forall \lambda \in S_{\theta, \omega}.$$

In fact, there is a useful condition on how to check, if a linear operator  $A$  is sectorial. It is given by the following proposition, which can be found in [38], Proposition 2.1.11, p.43:

**Proposition 2.19.** *Suppose  $A: D(A) \subset X \rightarrow X$  is a linear operator such that  $\rho(A)$  contains a half plane  $\{\lambda \in \mathbb{C} \mid \operatorname{Re} \lambda \geq \omega\}$ , and*

$$\|\lambda R(\lambda, A)\|_{L(X)} \leq M, \quad \text{if } \operatorname{Re} \lambda \geq \omega,$$

with  $\omega \in \mathbb{R}$  and  $M > 0$ . Then,  $A$  is sectorial.

If  $A$  is a sectorial operator, set  $e^{0A}x := x$  for all  $x \in X$  and define for  $t > 0$  the linear bounded operator  $e^{tA}$  by the Dunford integral

$$e^{tA} := \frac{1}{2\pi i} \int_{\omega + \gamma_{r, \eta}} e^{t\lambda} R(\lambda, A) d\lambda,$$

where  $r > 0$ ,  $\frac{\pi}{2} < \eta < \theta$  and  $\gamma_{r, \eta}$  is the curve  $\{\lambda \in \mathbb{C} \mid |\arg \lambda| = \eta, |\lambda| \geq r\} \cup \{\lambda \in \mathbb{C} \mid |\arg \lambda| \leq \eta, |\lambda| = r\}$ , oriented counterclockwise.

The family  $\{e^{tA} \mid t \geq 0\}$  of bounded linear operators is said to be the **analytic semi-group** generated by  $A$  on  $X$ .

In fact, it can be shown, that  $\lambda \mapsto e^{\lambda t}R(\lambda, A)$  is holomorphic in  $S_{\theta, \omega}$  and thus, the definition of  $e^{tA}$  is independent of  $r$  and  $\eta$ . Furthermore, the mapping  $t \mapsto e^{tA}$  is analytic from  $(0, \infty)$  to  $L(X)$  and it satisfies the semigroup property

$$e^{tA}e^{sA} = e^{(t+s)A}, \quad \forall s, t \geq 0,$$

see [38], chapter 2, for more information and proofs. Finally, it is

$$\lim_{t \rightarrow 0} e^{tA}x = x \iff x \in \overline{D(A)}.$$

If  $D(A)$  is dense in  $X$ , this is satisfied for all  $x \in X$ . Then  $\{e^{tA} \mid t \geq 0\}$  is said to be **strongly continuous**.

### 3 Modeling Liquid Phase Epitaxy: Physical Model and Two Scale Model

There are several approaches to model liquid phase epitaxy (LPE), as mentioned in the introduction. This thesis analyses a two scale model, proposed in [19]. In this chapter, the model is introduced. First, the non-homogenized model is presented in sections 3.1 and 3.2, and second, the two scale model in sections 3.3 and 3.4. The latter is derived from the non-homogenized model using homogenization techniques. The ansatz for the derivation is explained in section 3.3, but for technical details, the reader is referred to [19].

#### 3.1 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 4, and is filled with a liquid solution that contains the particles from which an epitaxial layer grows on a substrate, compare also Figures 2 and 3. 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  $Q^L(t) = Q \setminus \overline{Q^S(t)}$ .

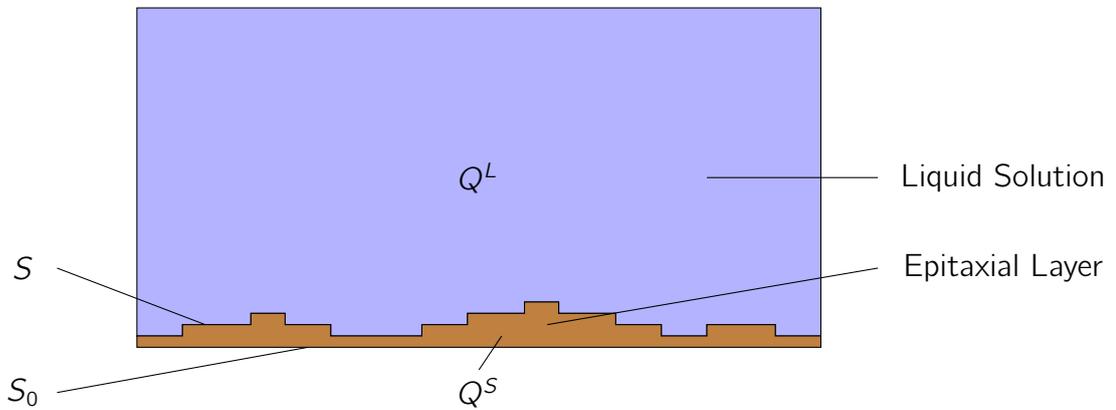


Figure 4: Liquid Phase Epitaxy.

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  $h: S_0 \rightarrow [0, \infty)$  over  $S_0$ :

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

and therefore

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

The process is modeled as step by step growth, see Figure 5(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 5(a). The union of these curves is denoted by  $\Lambda = \Lambda(t)$ .

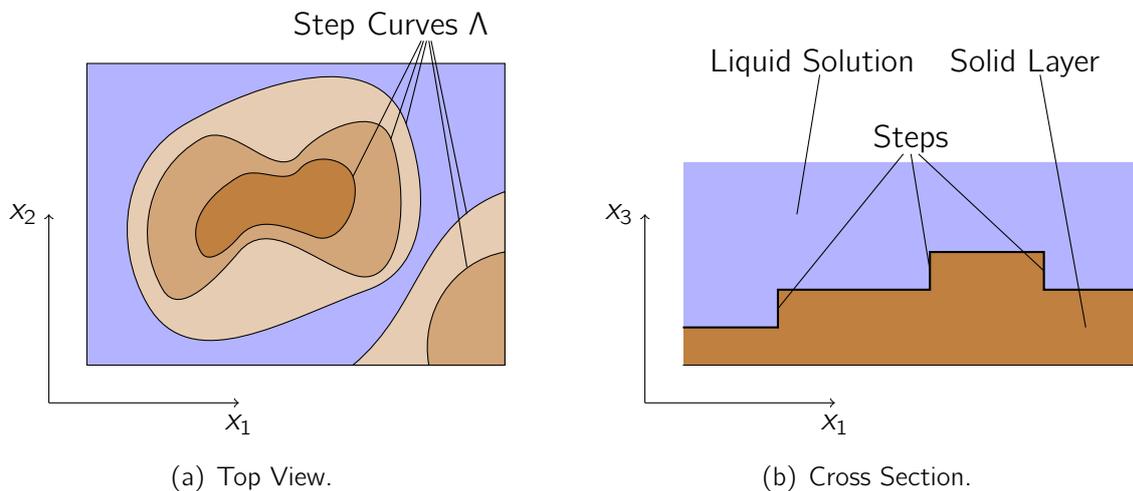


Figure 5: Step by Step Growth.

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

The processes to describe are, see Figure 6:

- 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, for further explanation see [19]:

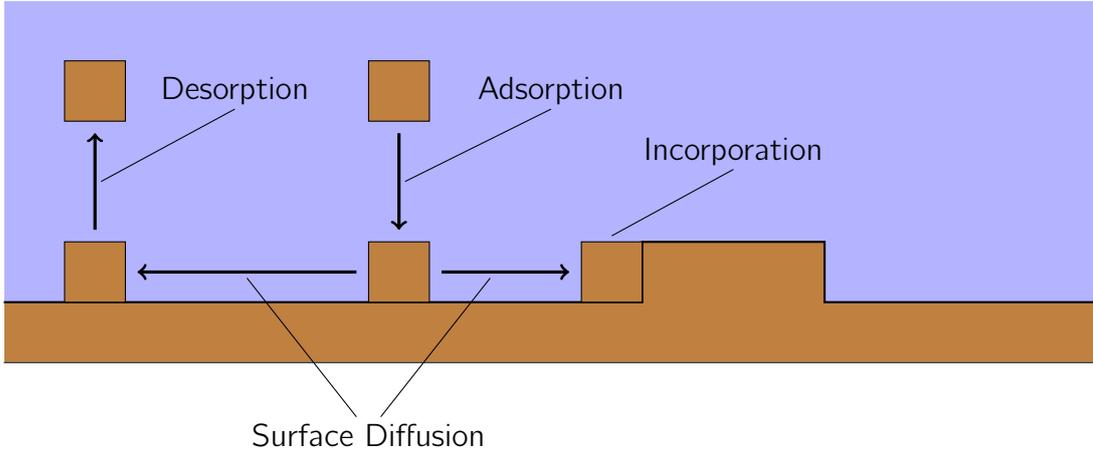


Figure 6: Processes in LPE.

- 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,

$$\begin{aligned} \operatorname{div} v &= 0, \\ \partial_t v + (v \cdot \nabla)v - \eta \Delta v + \nabla p &= 0, \end{aligned} \quad (3.1)$$

$$\partial_t c^\nu + v \cdot \nabla c^\nu - D^\nu \Delta c^\nu = 0, \quad (3.2)$$

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

Boundary conditions are

$$v = 0, \quad \text{on } \partial Q^L \setminus S, \quad (3.3)$$

$$v = J_S^{-1} \left( \frac{1}{\varrho^\nu} - \frac{1}{\varrho_E} \right) \left( \frac{c^\nu}{\tau^\nu} - \frac{c_s}{\tau_s} \right) n, \quad \text{on } S, \quad (3.4)$$

$$D^\nu \frac{\partial c^\nu}{\partial n} = 0, \quad \text{on } \partial Q^L \setminus S, \quad (3.5)$$

$$D^\nu \frac{\partial c^\nu}{\partial n} = J_S^{-1} (1 - c^\nu) \left( \frac{c_s}{\tau_s} - \frac{c^\nu}{\tau^\nu} \right), \quad \text{on } S, \quad (3.6)$$

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  $S_0$ ,  $\varrho^\nu$  and  $\varrho_E$  are the densities of the liquid solution and the solid layer respectively,  $\tau_s$  and  $\tau^\nu$  describe the rates of adsorption and desorption of adatoms from and to the liquid solution, and  $n = \frac{1}{\sqrt{1 + |\nabla h|^2}} ((\nabla h)^\top, -1)^\top$  is the outer normal on  $\partial Q^L$  at  $S$ . The coupling conditions (3.4) and (3.6) are derived under the assumption of conservation of the total mass and of the mass of adatoms, see [19], pp.4-5.

Furthermore, there are initial conditions

$$v(\cdot, 0) = v_{ini}, \quad c^{\mathcal{V}}(\cdot, 0) = c_{ini}^{\mathcal{V}}. \quad (3.7)$$

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

$$-\operatorname{div} \sigma(u) = 0, \quad \text{in } Q^S, \quad (3.8)$$

with displacement field  $u$ , stress tensor  $\sigma(u)$ , given by linear Hooke's 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

$$u = b, \quad \text{on } S_0. \quad (3.9)$$

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

$$\sigma(u)n - \eta e(v)n + pn = 0, \quad \text{on } S, \quad (3.10)$$

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

$$\sigma(u)n = 0, \quad \text{on } \partial Q^S \setminus (S_0 \cup S), \quad (3.11)$$

completes this part of the model.

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

$$\partial_t c_s = D_s \Delta c_s + \frac{c^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{c_s}{\tau_s}, \quad t \in I, x \in S_0 \setminus \Lambda(t), \quad (3.12)$$

$$c_s = c_{\text{eq}} \left( 1 + \frac{\kappa \gamma}{\varrho_s R T} \right) + \frac{h_A}{2RT} \sigma(u) : e(u), \quad t \in I, x \in \Lambda(t), \quad (3.13)$$

$$v_{\Lambda} = \frac{D_s}{\varrho_s} \left[ \frac{\partial c_s}{\partial n} \right], \quad t \in I, x \in \Lambda(t). \quad (3.14)$$

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,  $c_{\text{eq}}$  the equilibrium surface concentration at the monomolecular step,  $\kappa$  the curvature of the step,  $\gamma$  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  $v_{\Lambda}$

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  $\Lambda$ ,

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

where  $c_s^\pm = \lim_{r \rightarrow 0} c_s(x + rn^\pm)$  for  $x \in \Lambda$  with normal vector  $n^+ = n$  on  $\Lambda$  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 is the boundary condition

$$D_s \frac{\partial c_s}{\partial n} = 0, \quad \text{on } l \times \partial S_0, \quad (3.15)$$

and initial conditions

$$c_s(\cdot, 0) = c_{s,ini}, \quad \Lambda(0) = \Lambda_{ini}. \quad (3.16)$$

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

$$\partial_t h = \frac{1}{\rho E} \left( \frac{c^v}{\tau^v} - \frac{c_s}{\tau_s} \right), \quad (3.17)$$

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 [19] justify this by the fact, that the equations there are continuum 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.

## 3.2 Phase Field Approximation

Introduce a phase field function  $\phi: S_0 \rightarrow [0, \infty)$  which describes the height of the epitaxial film over a point on  $S_0$  by the number of monomolecular layers, see Figure 7. The use of the notion of "phase" and "phase field" expresses the mathematical similarity of what follows to diffuse interface models for solidification processes, see [9]. But 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

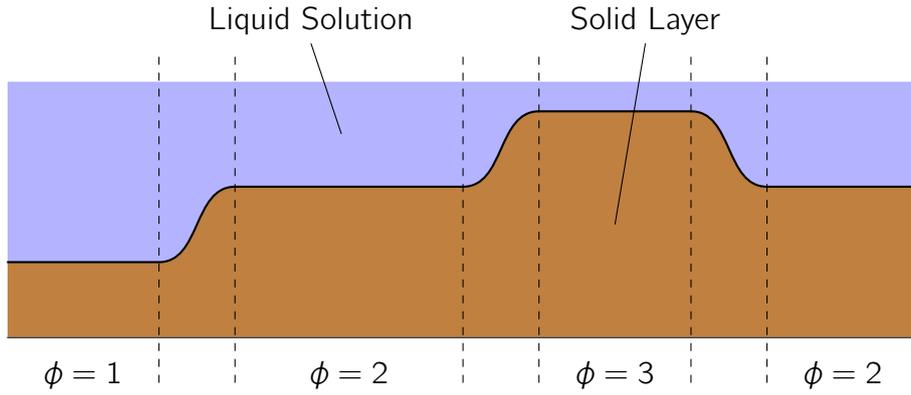


Figure 7: The Phase Field.

values of  $\phi$  would be the nonnegative integers, but  $\phi$  is allowed to take on real values in a neighborhood of a step which enables a smooth transition from step to step.

The BCF model (3.12) - (3.16) is replaced by a phase field approximation. It is derived from the free energy functional

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

with a multi-well potential  $f$  which has its minima at integer values, for example  $f(\phi) = -\cos(2\pi\phi)$ . The parameter  $\xi$  describes the thickness of the smooth transition regions. In [19] the functions  $g_1$  and  $g_2$  are chosen as  $g_1(\phi) = g_2(\phi) = \phi$ . Following the suggestions of [31] (where a model without elastic effects is discussed), another possible choice is

$$g_1(\phi) = \frac{1}{2} \left( \phi - \frac{\sin(2\pi\phi)}{2\pi} \right), \quad (3.18)$$

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

The parameter  $\beta$  is given by

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

where  $\varphi$ , which determines the shape of the diffuse transition region at a step, is the solution of

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

As in [9], the ansatz

$$\alpha \partial_t \phi = -D_\phi \mathcal{F}(\phi),$$

where  $\alpha$  is a relaxation parameter and  $D_\phi \mathcal{F}$  the Gâteaux derivative of  $\mathcal{F}$  with respect to  $\phi$ , leads to

$$\alpha \partial_t \phi = \frac{c_{\text{eq}} \gamma \beta}{\varrho_s} \left( \xi \Delta \phi - \frac{1}{\xi} f'(\phi) \right) + RT(c_s - c_{\text{eq}}) g'_1(\phi) - \frac{h_A}{2} \sigma(u) : e(u) g'_2(\phi)$$

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

$$\tau \xi^2 \partial_t \phi - \xi^2 \Delta \phi + f'(\phi) + q(\phi, c_s, u) = 0, \quad \text{in } I \times S_0, \quad (3.19)$$

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

$$q(\phi, c_s, u) = \frac{\xi RT \varrho_s}{c_{\text{eq}} \gamma \beta} (c_{\text{eq}} - c_s) g'_1(\phi) + \frac{\xi h_A \varrho_s}{2 c_{\text{eq}} \gamma \beta} \sigma(u) : e(u) g'_2(\phi). \quad (3.20)$$

With the choice of [19], the functions  $g'_1$  and  $g'_2$  are constant  $g'_1(\phi) = g'_2(\phi) = 1$ , while from (3.18), 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 chapter 5, both choices are allowed.  $\phi$  is endowed with an initial condition

$$\phi(\cdot, 0) = \phi_{\text{ini}}, \quad (3.21)$$

and a boundary condition

$$\frac{\partial \phi}{\partial n} = 0, \quad \text{on } I \times \partial S_0. \quad (3.22)$$

The surface diffusion equation (3.12) is modified to

$$\partial_t c_s + \varrho_s \partial_t \phi - D_s \Delta c_s = \frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} - \frac{c_s}{\tau_s}, \quad (3.23)$$

compare the corresponding equation in [9]. The additional term  $\varrho_s \partial_t \phi$  describes the conservation of adatoms.

The BCF model (3.12) - (3.14) can be interpreted as a sharp interface limit of (3.19), (3.23), see [17], [24], [31].

### 3.3 Ansatz for the Derivation of the 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. 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  $\varepsilon$ . Here,  $\varepsilon$  represents the scale of

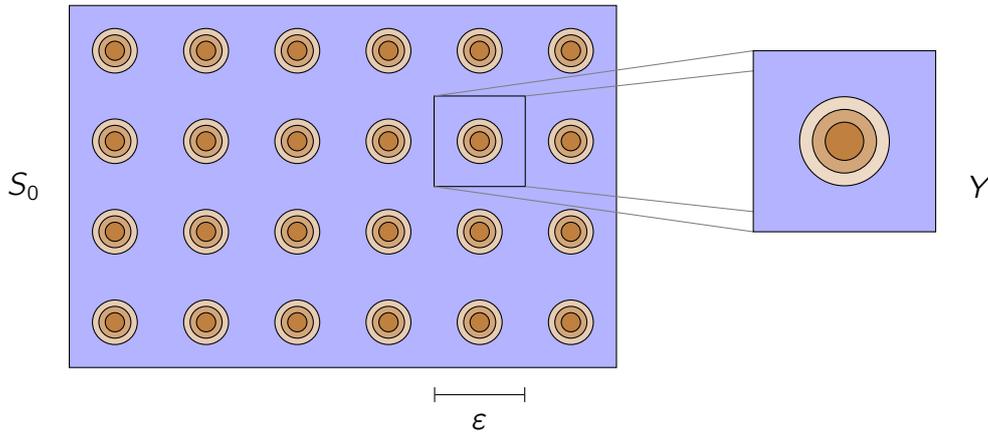


Figure 8: Periodic Homogenization in the  $x_1$ - $x_2$ -Plane.

the microstructure. In the following, the ansatz is explained and the resulting model is presented. For the technical details, see [19].

As ansatz it is assumed that the quantities in the physical model can be written as power series with respect to  $\varepsilon$ . 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 9. For the velocity field  $v$ , the pressure  $p$  and the volume concentration  $c^V$  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 outer expansions are

$$\begin{aligned} v_\varepsilon(x, t) &= V_0(x, t) + \varepsilon V_1(x, t) + \dots, \\ p_\varepsilon(x, t) &= P_0(x, t) + \varepsilon P_1(x, t) + \dots, \\ c_\varepsilon^V(x, t) &= \varepsilon C_0^V(x, t) + \varepsilon^2 C_1^V(x, t) + \dots, \end{aligned}$$

where the lower index  $\varepsilon$  indicates the problem of scale  $\varepsilon$ .

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 8. Therefore, asymptotic expansions for oscillations on the small scale  $\varepsilon$  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  $y_3 \rightarrow \infty$  has to be interpreted as the "border" between near and far field.

In the asymptotic expansions, the variable  $y$  is set to  $y = \frac{x}{\varepsilon}$ . The inner expansions in the fluid are

$$\begin{aligned} v_\varepsilon(x, t) &= v_0(x, t, \frac{x}{\varepsilon}) + \varepsilon v_1(x, t, \frac{x}{\varepsilon}) + \dots, \\ p_\varepsilon(x, t) &= p_0(x, t, \frac{x}{\varepsilon}) + \varepsilon p_1(x, t, \frac{x}{\varepsilon}) + \dots, \\ c_\varepsilon^V(x, t) &= \varepsilon c_0^V(x, t, \frac{x}{\varepsilon}) + \varepsilon^2 c_1^V(x, t, \frac{x}{\varepsilon}) + \dots \end{aligned}$$

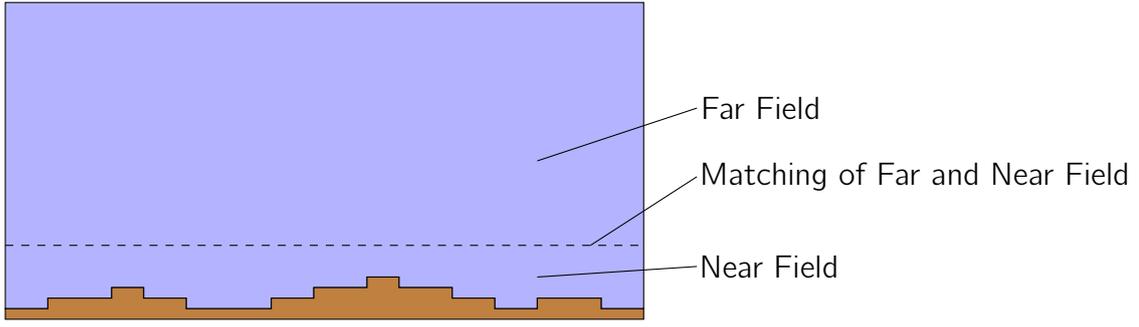


Figure 9: Inner and Outer Expansions.

For the elastic displacement, it is

$$u_\varepsilon(x, t) = \varepsilon u_0(x, t, \frac{x}{\varepsilon}) + \varepsilon^2 u_1(x, t, \frac{x}{\varepsilon}) + \dots,$$

for the surface concentration

$$c_{s,\varepsilon}(x, t) = \varepsilon c_{s,0}(x, t, \frac{x}{\varepsilon}) + \varepsilon^2 c_{s,1}(x, t, \frac{x}{\varepsilon}) + \dots,$$

and the height of the interface  $S$

$$h_\varepsilon(x, t) = \varepsilon h_0(x, t, \frac{x}{\varepsilon}) + \varepsilon^2 h_1(x, t, \frac{x}{\varepsilon}) + \dots$$

For the step boundaries  $\Lambda_\varepsilon$  at scale  $\varepsilon$ , it is assumed that

$$\Lambda_\varepsilon(t) = S_0 \cap \bigcup_{z \in M_Y} \varepsilon (z + \Lambda^\varepsilon(\varepsilon z, t)),$$

where  $M_Y$  is the set of shifts, see Definition 2.7. The surfaces  $\Lambda^\varepsilon(x, t) \subset Y$  depend in a suitable continuous sense on  $t$ ,  $x$  and  $\varepsilon$ . Furthermore is supposed, that there is some surface  $\Lambda^0(x, t)$  and a function  $\pi^\varepsilon(x, t, \cdot): \Lambda^0(x, t) \rightarrow Y$ , such that  $\Lambda^\varepsilon(x, t)$  converge to  $\Lambda^0(x, t)$  in some sense as  $\varepsilon \rightarrow 0$ , and

$$\Lambda^\varepsilon(x, t) = \{\pi^\varepsilon(x, t, y) \mid y \in \Lambda^0(x, t)\}.$$

Finally, for the velocity and curvature of the steps, it is assumed that

$$\begin{aligned} v_{\Lambda_\varepsilon} &= \varepsilon v_{\Lambda^0} + \varepsilon^2 v_{\Lambda^1} + \dots, \\ \kappa_\varepsilon &= \varepsilon^{-1} \kappa_0 + \varepsilon^0 \kappa_1 + \dots \end{aligned}$$

The quantities  $v_{\Lambda_\varepsilon}$  and  $\kappa_\varepsilon$  are evaluated at  $(x, t, \pi^\varepsilon(x, t, y))$ , while  $v_{\Lambda^i}$  and  $\kappa_i$  are evaluated at  $(x, t, y)$ , with  $y \in \Lambda^0(x, t)$ .

The above expansions already propose a scaling for the respective quantities. Furthermore, it is necessary to scale material parameters and given data in the inner expansions. The parameter scalings are

$$c_{eq} \sim \varepsilon, \quad h_A \sim \varepsilon, \quad \varrho_s \sim \varepsilon, \quad D_s \sim \varepsilon^2, \quad \gamma \sim \varepsilon^2.$$

The scale of all other parameters is  $\sim 1$ . As initial conditions is assumed that

$$v_\varepsilon(x, 0) = v_{ini}(x), \quad c_\varepsilon^Y(x, 0) = \varepsilon c_{ini}^Y(x), \quad c_{s,\varepsilon}(x, 0) = \varepsilon c_{s,ini}(x, \frac{x}{\varepsilon}), \quad x \in S_0,$$

with a given functions  $v_{ini}$ ,  $c_{ini}^Y$  and  $c_{s,ini}$ , where  $c_{s,ini}(x, y)$  is  $Y$ -periodic with respect to the second variable. For the boundary condition for  $u$  on  $S_0$ , it is supposed that

$$b_\varepsilon(x) = \varepsilon b_0(x, \frac{x}{\varepsilon}),$$

where  $b_0(x, y)$  also is  $Y$ -periodic with respect to the second variable.

The "homogenized" domain for the macroscopic space variable  $x$  is  $Q$ , see Figure 10, and for any  $x \in S_0$  there is a microscopic domain  $Y \times \mathbb{R}^+$ , which consist of the solid part

$$Q_Y^S(x, t) := \{y \in Y \times \mathbb{R}^+ \mid y_3 < h_0(x, t, y_1, y_2)\},$$

the liquid part

$$Q_Y^L(x, t) := \{y \in Y \times \mathbb{R}^+ \mid y_3 > h_0(x, t, y_1, y_2)\},$$

and the interface

$$S_Y(x, t) := \{y \in Y \times \mathbb{R}^+ \mid y_3 = h_0(x, t, y_1, y_2)\},$$

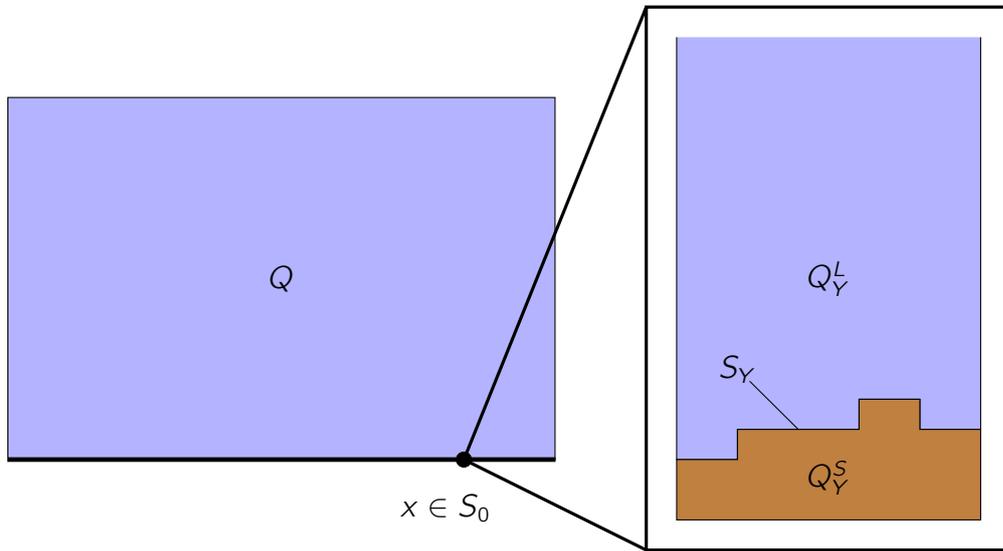


Figure 10: Macroscopic and Microscopic Domains.

The derivation of the two scale model works out as follows: Insert the above expansions into the model equations of section 3.1 and order by powers of  $\varepsilon$ . For most parts of the model, only the problems for the lowest order of  $\varepsilon$  are considered, see [19] for the precise derivation. The results are:

### The Equations in the Liquid Solution

For the lowest order of the outer expansions, the resulting system of differential equations is

$$\begin{aligned} \operatorname{div}_x V_0 &= 0, \\ \partial_t V_0 + (V_0 \cdot \nabla_x) V_0 - \eta \Delta_x V_0 + \nabla_x P_0 &= 0, \quad \text{in } I \times Q. \\ \partial_t C_0^\nu + V_0 \cdot \nabla_x C_0^\nu - D^\nu \Delta_x C_0^\nu &= 0, \end{aligned}$$

For the inner expansions the lowest order term of the velocity vanishes

$$v_0 \equiv 0,$$

and the lowest order term of the volume concentration is constant with respect to  $y$ . The matching between inner and outer expansions then leads to

$$\begin{aligned} V_0(x, t) &= 0, \\ c_0^\nu(x, t, y) &= C_0^\nu(x, t), \quad \text{on } I \times S_0, \end{aligned}$$

and further to

$$D^\nu \frac{\partial C_0^\nu}{\partial n} = \left( \frac{\bar{c}_{s,0}}{\tau_s} - \frac{C_0^\nu}{\tau^\nu} \right), \quad \text{on } I \times S_0,$$

where  $n = (0, 0, -1)^\top$  and  $\bar{c}_{s,0}(x, t) = \int_Y c_{s,0}(x, t, y) dy$  is the microscopic mean value of  $c_{s,0}$ . For the pressure it is

$$\lim_{y_3 \rightarrow \infty} p_0 = P_0.$$

In view of the elasticity problem, also the next order term  $v_1$  of the fluid velocity is needed, because it occurs there in a boundary condition. The corresponding equations for  $(x, t) \in S_0 \times I$  are

$$\begin{aligned} \operatorname{div}_y v_1 &= 0, \\ -\eta \Delta_y v_1 + \nabla_y p_0 &= 0, \quad \text{in } Q_Y^L(x, t), \end{aligned}$$

with the following condition at the interface  $S_Y$

$$v_1 = J_s^{-1} \left( \frac{1}{\rho^\nu} - \frac{1}{\rho^E} \right) \left( \frac{C_0^\nu}{\tau^\nu} - \frac{c_{s,0}}{\tau_s} \right) n, \quad \text{on } S_Y(x, t), \quad (3.24)$$

where  $n$  is the outer normal on  $Q_Y^L$  at  $S_Y$ . The matching to the outer expansion for  $v_1$  leads to

$$\lim_{y_3 \rightarrow \infty} e_y(v_1)(x, t, y) e_3 = e_x(V_0)(x, t) e_3, \quad \text{for } (x, t) \in S_0 \times I.$$

### The Equations in the Solid Domain

The leading order term solves for any  $(x, t) \in S_0 \times I$  the equation

$$-\operatorname{div}_y \sigma(u_0) = 0, \quad \text{in } Q_Y^S(x, t).$$

The boundary condition at  $S_Y(x, t)$  is

$$\sigma_y(u_0)n - \eta e_y(v_1)n + p_0 n = 0, \quad \text{on } S_Y(x, t).$$

### The Equations of the BCF Model

The lowest order terms solve for  $x \in S_0$  the equations

$$\begin{aligned} \partial_t c_{s,0} &= D_{s,0} \Delta_y c_{s,0} + \frac{C_0^V}{\tau^V} - \frac{c_{s,0}}{\tau_s}, & \text{in } I \times Y \setminus \Lambda^0(x, t), \\ c_{s,0} &= c_{\text{eq},0} \left( 1 + \frac{\kappa_0 \gamma_0}{\varrho_{s,0} R T} \right) + \frac{h_{A,0}}{2 R T} \sigma_y(u_0) : e_y(u_0), & \text{on } I \times \Lambda^0(x, t), \\ v_{\Lambda 0} &= \frac{D_{s,0}}{\varrho_{s,0}} \left[ \frac{\partial c_{s,0}}{\partial n} \right], & \text{on } I \times \Lambda^0(x, t). \end{aligned}$$

### The Phase Field Approximation of the BCF Model

Analogously to the explanations of section 3.2, also the two scale version of the BCF model can be replaced by a phase field approximation. It results in

$$\begin{aligned} \tau_0 \xi_0^2 \partial_t \phi_0 - \xi_0^2 \Delta_y \phi_0 + f'(\phi_0) + q_0(\phi_0, c_{s,0}, u_0) &= 0, \\ \partial_t c_{s,0} + \varrho_{s,0} \partial_t \phi_0 - D_{s,0} \Delta_y c_{s,0} &= \frac{C_0^V}{\tau^V} - \frac{c_{s,0}}{\tau_s}, \end{aligned} \quad \text{in } I \times Y,$$

with

$$q_0(\phi_0, c_{s,0}, u_0) = \frac{\xi_0 R T \varrho_{s,0}}{c_{\text{eq},0} \gamma_0 \beta} (c_{\text{eq},0} - c_{s,0}) g_1'(\phi_0) + \frac{\xi_0 h_{A,0} \varrho_{s,0}}{2 c_{\text{eq},0} \gamma_0 \beta} \sigma_y(u_0) : e_y(u_0),$$

and the scaled parameters  $\xi = \varepsilon \xi_0$  and  $\tau = \varepsilon^{-2} \tau_0$ .

### Use of the Phase Field for the description of the interface

The interpretation of the phase field is as already explained above: It denotes the number of monomolecular layers over a point  $y \in Y$ . This allows to replace the height function  $h_0$  for the description of the interface between solid layer and liquid solution. The thesis uses this approach and the microscopic domains are modified correspondingly, see Figure 11. That means that  $Q_Y^L$  is replaced by

$$Q_I(x, t) = \{y \in \mathbb{R}^3 \mid (y_1, y_2) \in Y, y_3 > h_{A,0} \phi_0(t, x, y_1, y_2)\},$$

$Q_Y^S$  by

$$Q_s(x, t) = \{y \in \mathbb{R}^3 \mid (y_1, y_2) \in Y, 0 < y_3 < h_{A,0}\phi_0(t, x, y_1, y_2)\},$$

and  $S_Y$  by

$$\Gamma(x, t) = \{y \in \mathbb{R}^3 \mid (y_1, y_2) \in Y, y_3 = h_{A,0}\phi_0(t, x, y_1, y_2)\}.$$

As simplification, the boundary condition (3.24) is replaced by

$$v_1 = - \left( \frac{1}{\rho_V} - \frac{1}{\rho_E} \right) \left( \frac{C_0^V}{\tau_V} - \frac{c_{s,0}}{\tau_S} \right) e_3, \quad \text{on } \Gamma.$$

This only is a modification at the steps. In fact it seems to be feasible from the physical point of view: The normal direction on  $\Gamma$  at a step is approximately perpendicular to the  $x_3$ -direction and since the height of a step is of the size of one particle diameter, there should not be a normal velocity of the fluid in that direction.

Concluding this chapter, the two scale model to be analyzed with completing boundary and initial conditions is summarized in the next section.

### 3.4 The Two Scale Model

The rest of this thesis is concerned with the following two scale model. In order to simplify the notation, the indices of the asymptotic expansions are omitted:

$v(x, t, y)$	$= v_1(x, t, y)$	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
$C^V(x, t)$	$= C_0^V(x, t)$	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

Capital letters denote purely macroscopic quantities, small letters indicate quantities depending on  $x$  and  $y$ . Also the index "0" for the parameters and the given data is omitted.

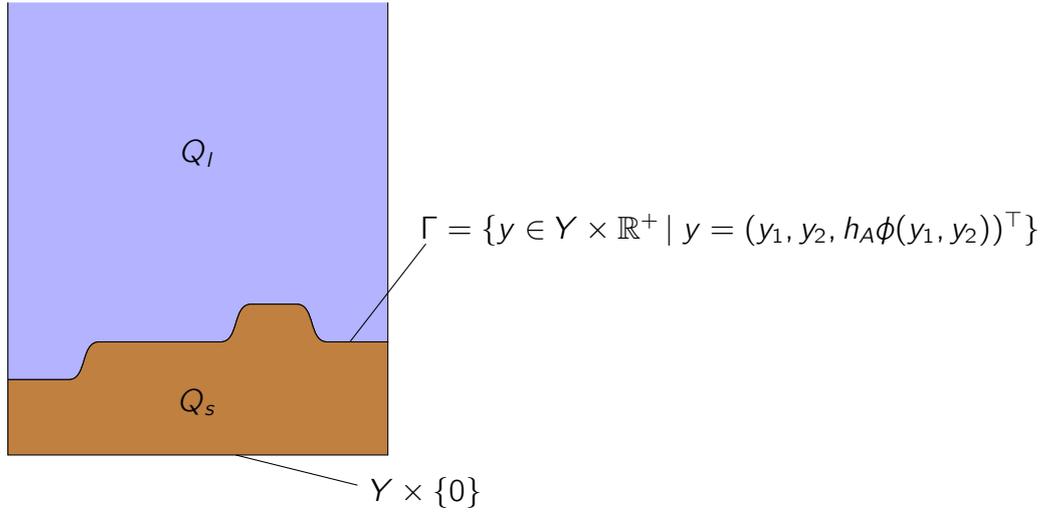


Figure 11: The Microscopic Interface and the Phase Field.

The model is composed of:

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

$$\begin{aligned} \operatorname{div}_x V &= 0, \\ \partial_t V + (V \cdot \nabla_x) V - \eta \Delta_x V + \nabla_x P &= 0, \end{aligned} \quad (3.25)$$

$$\partial_t C^\nu + V \cdot \nabla_x C^\nu - D^\nu \Delta_x C^\nu = 0. \quad (3.26)$$

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

$$D^\nu \frac{\partial C^\nu}{\partial n} = \left( \frac{\bar{c}_s}{\tau_s} - \frac{C^\nu}{\tau^\nu} \right), \quad (3.27)$$

$$V = 0, \quad (3.28)$$

where  $\bar{c}_s(x, t) = \int_Y c_s(x, t, y) dy$  is the microscopic mean value of  $c_s$ . Due to the boundary condition (3.28) the Navier-Stokes system (3.25) 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

$$\frac{\partial C^\nu}{\partial n} = 0, \quad (3.29)$$

$$V = 0, \quad (3.30)$$

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

$$C^\nu(0, x) = C_{ini}^\nu, \quad (3.31)$$

$$V(0, x) = V_{ini}. \quad (3.32)$$

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

$$\begin{aligned} \operatorname{div}_y v &= 0, \\ -\eta \Delta_y v + \nabla_y p &= 0, \end{aligned} \quad \text{in } Q_I, \quad (3.33)$$

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

$$v = v_\Gamma := - \left( \frac{1}{\varrho_V} - \frac{1}{\varrho_E} \right) \left( \frac{C^V}{\tau^V} - \frac{c_s}{\tau_s} \right) e_3. \quad (3.34)$$

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

$$\lim_{y_3 \rightarrow \infty} (\nabla_y v + (\nabla_y v)^\top) e_3 = (\nabla_x V|_{x_3=0} + (\nabla_x V)^\top|_{x_3=0}) e_3, \quad (3.35)$$

$$\lim_{y_3 \rightarrow \infty} p = P|_{x_3=0}. \quad (3.36)$$

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

$$-\operatorname{div}_y \sigma_y(u) = 0, \quad \text{in } Q_s, \quad (3.37)$$

This system is completed by a Dirichlet boundary condition

$$u = b, \quad \text{for } y \in \tilde{\Gamma} := Y \times \{0\}, \quad (3.38)$$

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

$$\sigma_y(u)n - \eta e_y(v)n + pn = 0, \quad \text{on } \Gamma, \quad (3.39)$$

to the Stokes system. Here  $n$  is the outer normal vector on  $Q_s$  at  $\Gamma$ .

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

$$\tau \xi^2 \partial_t \phi - \xi^2 \Delta_y \phi + f'(\phi) + q(\phi, c_s, u) = 0, \quad (3.40)$$

$$\partial_t c_s + \varrho_s \partial_t \phi - D_s \Delta_y c_s = \frac{C^V}{\tau^V} - \frac{c_s}{\tau_s}, \quad (3.41)$$

with  $Y$ -periodic initial conditions

$$c_s(0, x, y) = c_{s,ini}(x, y), \quad \phi(0, x, y) = \phi_{ini}(x, y), \quad (3.42)$$

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

$$q(\phi, c_s, u) = \frac{\xi R T \varrho_s}{c_{eq} \gamma \beta} (c_{eq} - c_s) g'_1(\phi) + \frac{\xi h_A \varrho_s}{2 c_{eq} \gamma \beta} \sigma_y(u) : e_y(u), \quad (3.43)$$

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 [31] and ensures that the corresponding term is only nonzero in the neighborhood of a step, while the second is that of [19].

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 [42], where only few selected microscopic problems are solved, might be applicable: It requires continuous interscale dependencies, which are proven in sections 5.2.4 and 5.3. This reduces the computation effort significantly.

The above model is a first try to include elastic effects into the model of [10] and [17] without elasticity, for which existence and uniqueness of solutions is proven, the formal derivation of the two scale model is justified rigorously, for both see [17], and numerical experiments are presented with good results, see [10]. This thesis proves existence and uniqueness of solutions for the extended model, but several questions are still open, especially the justification of the homogenization approach, and numerical experiments are still missing.

Also concerning the model, there is room for discussion. It is not clear, for example, how to model the misfit between substrate and layer correctly. In [19], as in most foregone models, this is done as prescribed stress of the form

$$\sigma(u)n = b, \quad \text{on } Y \times \{0\}, \quad (3.44)$$

while here, a prescribed displacement is assumed, see condition (3.38). The latter ensures uniqueness of the solution of the elasticity problem, while a solution for the Neumann condition (3.44) in combination with the Neumann condition (3.39) 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, [48]. 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 with the elasticity. From the interpretation of  $\phi$ , 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 (3.43). Furthermore, if the phase field is zero, the elastic energy term in (3.43) 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 (3.43) and to multiply the elastic term by a function  $g'_2(\phi)$  which becomes zero for  $\phi \in \mathbb{N}_0$ , for

example

$$g'_2(\phi) = \frac{1}{2}(1 - \cos(2\pi\phi)),$$

compare  $g_1$  in (3.18). The analysis of chapter 5 covers this choice, too.



## 4 An Iterative Solving Procedure

In the following, an iterative solving procedure for the two scale model of chapter 3 is proposed. It can be a basis for both - analysis and numerics. Actually, the strategy of the proof of the main solvability result (Theorem 5.1) in chapter 5 reflects the following iteration. Conversely, the results of chapter 5 substantiate the iteration and even ensure its convergence, see Theorem 4.1. All of its assumptions are verified in chapter 5. 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 2.18.

Due to to the boundary condition (3.28) the Navier–Stokes system decouples from the rest of the model equations. As a consequence the macroscopic velocity  $V$  and the macroscopic pressure  $P$  can be computed in advance. The subsequent iterative procedure consists in fact of two encapsulated iterations: The remaining macroscopic convection–diffusion equation and the coupled microscopic problem (composed of phase field, Stokes and Elasticity system) are solved in turns (outer iteration) where in each step, the microscopic problem is again solved iteratively (inner iteration), see Figure 12.

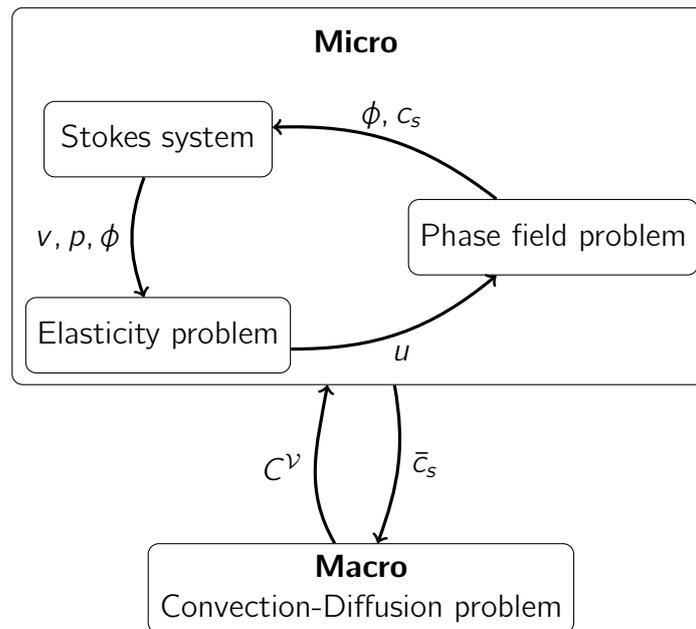


Figure 12: Encapsulated Fixed Point Iterations.

More precisely: Suppose that each single microscopic problem has a unique solution for given coupling data and denote by  $\mathcal{S}_{\text{Stokes}}$ ,  $\mathcal{S}_{\text{elastic}}$  and  $\mathcal{S}_{\text{phasefield}}$  the corresponding solution operators, compare section 5.2.4. Assume furthermore, that there exists for given  $C^V$  a unique solution of the coupled microscopic problem and for given  $c_s$  an unique solution of the macroscopic problem with solution operators  $\mathcal{L}_{\text{micro}}$  and  $\mathcal{L}_{\text{macro}}$  respectively, compare section 5.4.

Then, the iteration reads:

1. Solve the decoupled macroscopic Navier–Stokes system (3.25), (3.28), (3.30), (3.32) 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  $C_0^\nu(t) \equiv C_{ini}^\nu$ ,  $c_{s,0}(t) \equiv c_{s,ini}$  and  $\phi_0(t) \equiv \phi_{ini}$ , for all  $t \in I$ .
3. Choose a tolerance  $\text{tol} > 0$ , in order to set an abort criterion for the inner iteration.
4. Solve the microscopic equations, with macroscopic coupling datum  $C_0^\nu$ , 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 (3.33), (3.34), (3.35).
  - (b) Solve the microscopic elasticity system (3.37), (3.38), (3.39) with data  $v^0, p^0$  and  $\phi^0$  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 (3.40), (3.41), (3.42) with coupling datum  $u^0$ .
  - (d) Restart in 4.(a) with  $\phi^1$  and  $c_s^1$  instead of  $\phi^0$  and  $c_s^0$ . Continue the microscopic iteration, until  $\|(\phi^N, c_s^N) - \mathcal{L}_{\text{micro}}(C_0^\nu)\| < \text{tol}$ .
5. Set  $c_{s,1} := c_s^N$  and  $\phi_1 := \phi^N$ . Solve the macroscopic convection–diffusion problem (3.26), (3.27), (3.29), (3.31) to get  $C_1^\nu := \mathcal{L}_{\text{macro}}(\phi_1, c_{s,1})$ .
6. Restart in 4. with data  $C_1^\nu, c_{s,1}$  and  $\phi_1$  instead of  $C_0^\nu, c_{s,0}$  and  $\phi_0 \dots$

In chapter 5, existence and uniqueness of solutions of each single problem is proven in suitable function spaces, if the coupling data is supposed to be given. This ensures that the corresponding solution operators exist and every step in the above iteration is meaningful. Furthermore, the fixed point operators

$$\begin{aligned} \mathcal{S} &:= \mathcal{S}_{\text{phasefield}} \circ \mathcal{S}_{\text{elastic}} \circ \mathcal{S}_{\text{Stokes}} : & (\tilde{\phi}, \tilde{c}_s) &\mapsto (\phi, c_s), \\ \mathcal{L} &:= \mathcal{L}_{\text{macro}} \circ \mathcal{L}_{\text{micro}} : & \tilde{C}^\nu &\mapsto C^\nu, \end{aligned}$$

are investigated, 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

$$\begin{aligned} \|\mathcal{S}(\phi, c_s) - \mathcal{S}(\tilde{\phi}, \tilde{c}_s)\|_1 &\leq k_1 \|(\phi, c_s) - (\tilde{\phi}, \tilde{c}_s)\|_1, \\ \|\mathcal{L}(C^\nu) - \mathcal{L}(\tilde{C}^\nu)\|_2 &\leq k_2 \|C^\nu - \tilde{C}^\nu\|_2, \end{aligned}$$

with suitable norms  $\|\cdot\|_1$  and  $\|\cdot\|_2$ . In chapter 5, these norms will be chosen as

$$\begin{aligned}\|(\phi, c_s)\|_1 &= \|\phi\|_{C^\alpha(I, C^2(\Upsilon))} + \|c_s\|_{C^\alpha(I, C^2(\Upsilon))}, \\ \|C^\mathcal{V}\|_2 &= \|C^\mathcal{V}\|_{C(I, W_{r_2}^1(Q))} + \|C^\mathcal{V}\|_{C^1(I, (W_{r_2'}^1(Q)))}.\end{aligned}$$

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*

$$\|C_n^\mathcal{V} - C_*^\mathcal{V}\|_2 \leq \frac{L \cdot \text{tol}}{1 - k_2} + \frac{k_2^n}{1 - k_2} \|\mathcal{L}(C_0^\mathcal{V}) - C_0^\mathcal{V}\|_2.$$

Thus, the iteration converges to  $C_*^\mathcal{V}$  for  $\text{tol} \rightarrow 0$  and  $n \rightarrow \infty$ .

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

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

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

$$\tilde{C}_0^\mathcal{V} := C_0^\mathcal{V}, \quad \tilde{C}_{n+1}^\mathcal{V} := \mathcal{L}(\tilde{C}_n^\mathcal{V}), \quad n \in \mathbb{N}_0,$$

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

$$\|\tilde{C}_n^\mathcal{V} - C_*^\mathcal{V}\|_2 \leq \frac{k_2^n}{1 - k_2} \|\mathcal{L}(C_0^\mathcal{V}) - C_0^\mathcal{V}\|_2. \quad (4.1)$$

In any step of the iteration, it is

$$\begin{aligned}\|C_{n+1}^\mathcal{V} - \mathcal{L}(C_n^\mathcal{V})\|_2 &= \|\mathcal{L}_{\text{macro}}(\phi_{n+1}, c_{s,n+1}) - \mathcal{L}_{\text{macro}}(\mathcal{L}_{\text{micro}}(C_n^\mathcal{V}))\|_2 \\ &\leq L \|(\phi_{n+1}, c_{s,n+1}) - \mathcal{L}_{\text{micro}}(C_n^\mathcal{V})\|_1 \\ &\leq L \cdot \text{tol}.\end{aligned}$$

It follows that

$$\begin{aligned}\|C_{n+1}^{\mathcal{V}} - \tilde{C}_{n+1}^{\mathcal{V}}\|_2 &\leq \|C_{n+1}^{\mathcal{V}} - \mathcal{L}(C_n^{\mathcal{V}})\|_2 + \|\mathcal{L}(C_n^{\mathcal{V}}) - \mathcal{L}(\tilde{C}_n^{\mathcal{V}})\|_2 \\ &\leq L \cdot \text{tol} + k_2 \|C_n^{\mathcal{V}} - \tilde{C}_n^{\mathcal{V}}\|_2,\end{aligned}$$

and finally, due to  $C_0^{\mathcal{V}} = \tilde{C}_0^{\mathcal{V}}$ ,

$$\|C_{n+1}^{\mathcal{V}} - \tilde{C}_{n+1}^{\mathcal{V}}\|_2 \leq L \cdot \text{tol}(1 + k_2 + \dots + k_2^n) \leq \frac{L \cdot \text{tol}}{1 - k_2}. \quad (4.2)$$

The combination of (4.1) and (4.2) proves the result.  $\square$

## 5 Existence and Uniqueness of Solutions of the Two Scale Model

Chapter 5 is the core of this thesis. The well-posedness of the two scale model is investigated here, and existence and uniqueness of solutions are proven as main result. First, in 5.1, the solvability result is formulated in Theorem 5.1, without giving a proof, supplemented with some remarks.

A proof is presented in the subsequent sections 5.2, 5.3 and 5.4. The rough strategy is already indicated in chapter 4, see Figure 12: 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.

### 5.1 The Main Result

As already mentioned in section 3, the Navier-Stokes problem decouples from the rest of the model, due to condition (3.28). 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 thesis. In the textbooks [26], [52], 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 (3.33), (3.34), (3.35) and the elastic problem (3.37), (3.38), (3.39) 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  $Q_I = Q_I(t)$  and  $Q_S = Q_S(t)$ , but on time independent domains  $\hat{Q}_I$  and  $\hat{Q}_S$ . The corresponding (time dependent) domain transformations are denoted by

$$\Psi_I(t): \hat{Q}_I \rightarrow Q_I(t), \quad \Psi_S(t): \hat{Q}_S \rightarrow Q_S(t).$$

The technical details are described in sections 5.2.1 and 5.2.2. For functions  $v$ ,  $p$  and  $u$ , defined on  $Q_I(t)$  and  $Q_S(t)$  respectively,  $\hat{v} := v \circ \Psi_I$ ,  $\hat{p} := p \circ \Psi_I$  and  $\hat{u} := u \circ \Psi_S$  denote their counterparts, defined on the time-independent domains  $\hat{Q}_I$  and  $\hat{Q}_S$ .

The theorem reads:

**Theorem 5.1** (Existence and uniqueness of solutions of the fully coupled problem). *Suppose  $V \in C^\beta(I, C(\overline{Q})) \cap C(I, C^1(\overline{Q}))$ , for some  $\beta > 0$ , and  $P \in C(I \times \overline{Q})$  are solutions of the Navier-Stokes equations (3.25), (3.28), (3.30) and (3.32). Assume furthermore that  $\phi_{ini}, c_{s,ini} \in C(S_0, C_{\text{per}}^{2+2\alpha}(Y))$ , with  $\phi_{ini}(y) > 0$  for all  $y \in \overline{Y}$ ,  $b \in C(I \times S_0, W_{r_1, \text{per}}^{2-1/r_1}(\tilde{\Gamma}))$  and  $C_{ini}^\nu \in W_{r_2}^1(Q)$ , 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 (3.26), (3.27), (3.29), (3.31) and (3.33) – (3.42) in the following function spaces:*

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

**Some remarks:**

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

**On the condition  $\phi_{ini} > 0$ :** The condition  $\phi(t, y) > 0$  is needed in the analysis for the elasticity problem. It ensures that the domain  $Q_s$  does not form any cusps and that  $\Psi_s$  and  $\hat{Q}_s$  can be defined as described in section 5.2.2. And  $\phi_{ini}(y) > 0$  implies that  $\phi(t, y)$  remains positive for small enough  $t > 0$ .

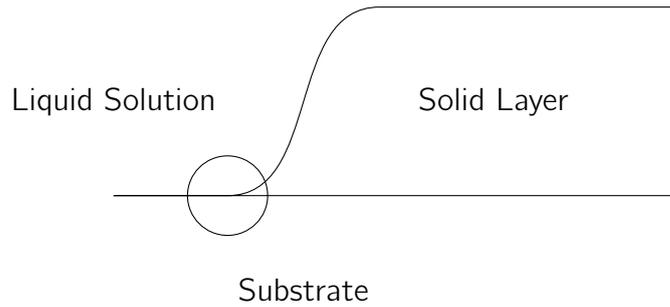


Figure 13: A Cusp in the Solid Domain if  $\phi$  becomes zero.

**On the length  $\tau_0$  of the time interval of existence:** Theorem 5.1 proves existence of solutions of the model only on a local time interval  $[0, \tau_0]$ . Its length  $\tau_0$  depends principally on the given data and the constants in the a priori and continuity estimates of the single parts of the problem. If these values are supposed to be known, the size of  $\tau_0$  can be calculated explicitly, following the proofs in the coming sections.

**On the well-posedness:** It is possible to adapt the proofs in the following sections to show, that the solution of the two scale model depends continuously on  $V$ ,  $P$  and initial and coupling data. So the problem is well-posed in the sense of Hadamard, [28].

## 5.2 Solvability of the Microscopic Equations

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  $C^\nu(x, \cdot), V(x, \cdot), P(x, \cdot) \in C(I)$ . These macroscopic quantities at a fixed point  $x \in S_0$  are constant with respect to  $y$ .

First, the single problems are discussed in sections 5.2.1–5.2.3, section 5.2.4 studies the microscopic coupling.

Concerning the notation: In some of the following estimates, the constant depends on the boundary of the corresponding domain and thus on  $\phi$  (sometimes on two phase fields  $\phi_1$  and  $\phi_2$ ). It is stated explicitly in these cases. Mostly, this dependency will be expressed in terms of an upper bound  $\kappa$  which satisfies

$$\kappa \geq \|\phi\|_{C(I, C^2(Y))} \quad \text{or} \quad \kappa \geq \max\{\|\phi_1\|_{C(I, C^2(Y))}, \|\phi_2\|_{C(I, C^2(Y))}\}, \quad (5.1)$$

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

### 5.2.1 The Microscopic Stokes System

Consider (3.33), (3.34) and (3.35). The discussion of this part of the model is organized as follows: First, look for solutions of the problem on the semi-infinite domain  $Q_I$  in suitable Hilbert spaces, and second, discuss the regularity of this solution on a bounded subdomain  $Q_{IK} \subset Q_I$ , which is defined in (5.2). 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  $\Gamma$ .

Condition (3.35) reads

$$\begin{aligned} \lim_{y_3 \rightarrow \infty} (\nabla_y v + (\nabla_y v)^\top) e_3 &= (\nabla_x V + (\nabla_x V)^\top) e_3 \\ &= (\partial_{x_3} V_1, \partial_{x_3} V_2, 0)^\top \\ &=: \mathbf{a}, \end{aligned}$$

using the boundary condition (3.28), which leads to  $\partial_{x_1} V = \partial_{x_2} V = 0$  and implies together with  $\operatorname{div} V = 0$  that  $\partial_{x_3} V_3 = 0$ , for  $x \in S_0$ . For some sufficiently large constant  $M > h_A \|\phi\|_{L^\infty(Y)}$ , define

$$\tilde{v} = \begin{cases} 0, & \text{für } y_3 \leq M, \\ \zeta(y_3) \mathbf{a} & \text{für } M < y_3 < M + 1, \\ \mathbf{a}(y_3 - M) & \text{für } y_3 \geq M + 1, \end{cases}$$

with a function  $\zeta$  that satisfies

$$\zeta(M) = 0, \quad \zeta'(M) = 0, \quad \zeta''(M) = 0, \quad \zeta(M+1) = 1, \quad \zeta'(M+1) = 1, \quad \zeta''(M+1) = 0,$$

for example  $\zeta(y_3) = 3(y_3 - M)^5 - 8(y_3 - M)^4 + 6(y_3 - M)^3$ . Then  $\tilde{v}$  is two times continuously differentiable with

$$\lim_{y_3 \rightarrow \infty} (\nabla_y \tilde{v} + (\nabla_y \tilde{v})^\top) e_3 = \mathbf{a},$$

$$\Delta \tilde{v} = \begin{cases} 0, & \text{für } y_3 \leq M, \\ \zeta''(y_3) \mathbf{a} & \text{für } M < y_3 < M + 1, \\ 0 & \text{für } y_3 \geq M + 1. \end{cases}$$

Since the third component of  $\mathbf{a}$  (and thus of  $\tilde{v}$ ) vanishes,  $\tilde{v}$  is divergence-free:

$$\operatorname{div} \tilde{v} = 0, \quad \text{for all } y \in Q_I.$$

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

$$\int_\Gamma \bar{v} \cdot n \, dy = \int_\Gamma v_\Gamma \cdot n \, dy, \quad \text{i.e.} \quad \bar{v}_3 := \frac{\int_\Gamma v_\Gamma \cdot n \, dy}{\int_\Gamma n_3 \, dy},$$

where  $v_\Gamma$  is given by (3.34). Introduce an artificial boundary  $\hat{\Gamma} := \{y \in Q_I \mid y_3 = h_A \phi(y_1, y_2) + K\}$ , with some positive constant  $K$ . The surface  $\hat{\Gamma}$  is the upper boundary of the bounded domain

$$Q_{IK} := \{y \in Q_I \mid y_3 < h_A \phi(y_1, y_2) + K\}. \quad (5.2)$$

As already mentioned in section 5.1, the transformation of  $Q_I$  and  $Q_{IK}$  into time independent domains is needed. Thus, define  $\hat{Q}_I := Y \times (0, \infty)$ ,  $\hat{Q}_{IK} := Y \times (0, K)$  and

$$\text{or } \left. \begin{array}{l} \Psi_I(t): \hat{Q}_I \rightarrow Q_I(t): \\ \Psi_{IK}(t): \hat{Q}_{IK} \rightarrow Q_{IK}(t): \end{array} \right\} \hat{y} = \begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \end{pmatrix} \mapsto y := \begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 + h_A \phi(t, \hat{y}_1, \hat{y}_2) \end{pmatrix}. \quad (5.3)$$

The following Lemma guaranties that the inhomogeneous Dirichlet condition (3.34) on  $\Gamma$  can be transformed into a homogeneous one:

**Lemma 5.2.** *Suppose that  $Y = [0, 1]^2$ . Then, there exists a function  $u \in [H_{\text{per}}^1(Q_{IK})]^3$  such that  $u|_\Gamma = v_\Gamma - \bar{v}$ ,  $u|_{\hat{\Gamma}} = 0$  and  $\operatorname{div} u = 0$ . Furthermore,*

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

*Proof.* In a **first step**, consider the time independent domain  $\hat{Q}_{IK}$  and the transformation  $\Psi_{IK}(t): \hat{Q}_{IK} \rightarrow Q_{IK}(t)$ . A vector field on  $Q_{IK}$  is transformed into a vector field on  $\hat{Q}_{IK}$  by using the Piola transform for vectors, which is defined for fixed  $\hat{y} \in \hat{Q}_{IK}$ ,  $y = \Psi_{IK}(\hat{y}) \in Q_{IK}$  by

$$\mathcal{P}: \mathbb{R}^3 \rightarrow \mathbb{R}^3: v(y) \mapsto v^{\mathcal{P}}(\hat{y}) := \operatorname{Cof}(D\Psi_{IK}(\hat{y}))^\top v(y),$$

where  $\text{Cof}(D\Psi_I(\hat{y}))^\top$  is the transposed of the Cofactor matrix of  $D\Psi_I(\hat{y})$ :

$$D\Psi_I(\hat{y}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ h_A \partial_{\hat{y}_1} \phi(\hat{y}_1, \hat{y}_2) & h_A \partial_{\hat{y}_2} \phi(\hat{y}_1, \hat{y}_2) & 1 \end{pmatrix},$$

$$\text{Cof}(D\Psi_I(\hat{y})) = \begin{pmatrix} 1 & 0 & -h_A \partial_{\hat{y}_1} \phi(\hat{y}_1, \hat{y}_2) \\ 0 & 1 & -h_A \partial_{\hat{y}_2} \phi(\hat{y}_1, \hat{y}_2) \\ 0 & 0 & 1 \end{pmatrix}.$$

The Piola transform has the property that

$$\text{div}_{\hat{y}} v^{\mathcal{P}} = \det(D\Psi_I) \text{div}_y v = \text{div}_y v, \quad \int_{\partial \hat{Q}_{IK}} v^{\mathcal{P}} \cdot n \, d\hat{s} = \int_{\partial Q_{IK}} v \cdot n \, ds,$$

see e.g. [45], Ch.1.4. Prove now, that there exists a function  $w^{\mathcal{P}} \in [H_{\text{per}}^1(\hat{Q}_{IK})]^3$  such that  $w^{\mathcal{P}}|_{y_3=0} = (v_\Gamma - \bar{v})^{\mathcal{P}}$  and  $w^{\mathcal{P}}|_{y_3=K} = 0$ . Therefore, consider the following boundary value problem

$$\Delta w^{\mathcal{P}} = 0, \quad \text{in } \hat{Q}_{IK}, \quad (5.4)$$

$$w^{\mathcal{P}} = \begin{cases} 0 & \text{for } \hat{y}_3 = K, \\ (v_\Gamma - \bar{v})^{\mathcal{P}} & \text{for } \hat{y}_3 = 0, \\ Y\text{-periodic} & \text{with respect to } (\hat{y}_1, \hat{y}_2) \in Y. \end{cases} \quad (5.5)$$

Since  $v_\Gamma \in H_{\text{per}}^{1/2}(\Gamma)$ , the function  $(v_\Gamma - \bar{v})^{\mathcal{P}}$  can be expanded into a Fourier series

$$(v_\Gamma - \bar{v})^{\mathcal{P}}(y_1, y_2) = \sum_{k,l \in \mathbb{Z}} c_{kl} e^{2\pi i(ky_1 + ly_2)},$$

where the coefficients  $c_{kl}$  satisfy

$$\sum_{k,l \in \mathbb{Z}} |c_{kl}|^2 (1 + k^2 + l^2)^{\frac{1}{2}} < \infty. \quad (5.6)$$

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

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

Then,  $w^{\mathcal{P}}$  is a solution of (5.4), if the coefficients  $b_{kl}$  solve the ordinary differential equation

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

with boundary conditions

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

Hence

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

where

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

The condition  $w^{\mathcal{P}} \in H^1(\hat{Q}_{IK})$  is equivalent to

$$\sum_{k,l \in \mathbb{Z}} \|b_{kl}\|_{L_2(0,K)}^2 (1 + k^2 + l^2) < \infty \quad \text{and} \quad \sum_{k,l \in \mathbb{Z}} \|b'_{kl}\|_{L_2(0,K)}^2 < \infty.$$

This can be verified by basic calculations using (5.6). These calculations also lead to the estimate

$$\|w^{\mathcal{P}}\|_{H^1(\hat{Q}_{IK})} \leq c \|(v_{\Gamma} - \bar{v})^{\mathcal{P}}\|_{H^{1/2}(Y)} \leq c (1 + \|\phi\|_{C^2(Y)}) \|v_{\Gamma} - \bar{v}\|_{H^{1/2}(Y)}. \quad (5.7)$$

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

**Second step:** Prove the existence of a divergence free function in  $H_{\text{per}}^1(\hat{Q}_{IK})$  with boundary values (5.5). From the construction of  $\bar{v}$ , the periodicity of  $w^{\mathcal{P}}$  and the properties of the Piola transform it follows

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

Follow the ideas of [26], Ch.I, §2.2 and get a function  $v^{\mathcal{P}} \in [H_0^1(\hat{Q}_{IK})]^3$  with

$$\operatorname{div} v^{\mathcal{P}} = \operatorname{div} w^{\mathcal{P}}, \quad \|\nabla v^{\mathcal{P}}\|_{L_2(\hat{Q}_{IK})} \leq c \|\operatorname{div} w^{\mathcal{P}}\|_{L_2(\hat{Q}_{IK})}. \quad (5.8)$$

Since all functions in  $[H_0^1(\hat{Q}_{IK})]^3$  are  $Y$ -periodic, this is also true for  $v^{\mathcal{P}}$  and thus also for  $u^{\mathcal{P}} := w^{\mathcal{P}} - v^{\mathcal{P}}$ . Estimates (5.7), (5.8) and Poincaré's inequality, see (2.5), for  $v^{\mathcal{P}}$  imply

$$\|u^{\mathcal{P}}\|_{H^1(\hat{Q}_{IK})} \leq c (1 + \|\phi\|_{C^2(Y)}) \|v_{\Gamma} - \bar{v}\|_{H^{1/2}(Y)}. \quad (5.9)$$

The constant occurring in Poincaré's inequality only depends on the diameter of  $\hat{Q}_{IK}$ . Thus the constant  $c$  in (5.9) is independent of  $u^{\mathcal{P}}$ ,  $v_{\Gamma}$  and  $\phi$ .

**Third and last step:** Use the inverse Piola transform to define

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

This is the required function which satisfies the boundary conditions and is divergence free by construction. The product and the chain rule imply  $u \in [H_{\text{per}}^1(Q_{IK})]^3$  with

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

□

Extend  $u$  to  $Q_I$  by setting  $u(y) = 0$  for  $y \in Q_I \setminus Q_{IK}$ . Obviously,  $u \in [H_{\text{per}}^1(Q_I)]^3$  with  $\text{div } u = 0$ . Return to the Stokes problem (3.33), (3.34), (3.35). For the function  $z := v - \bar{v} - \tilde{v} - u$  consider the problem

$$\begin{aligned} -\eta \Delta z + \nabla p &= \eta (\Delta u + \Delta \tilde{v}), \\ \text{div } z &= 0, \end{aligned} \quad \text{in } Q_I, \quad (5.10)$$

with

$$z = 0 \quad \text{on } \Gamma, \quad \lim_{y_3 \rightarrow \infty} e(z)e_3 = 0, \quad z \text{ is } Y\text{-periodic}, \quad (5.11)$$

where  $e(z) = \frac{1}{2}(\nabla z + (\nabla z)^\top)$ . If  $z$  solves (5.10), then  $v$  is a solution of the original problem (3.33). Set

$$\mathcal{X} := \left\{ w|_{Q_I} \mid w(\cdot, \cdot, y_3) \in C_{\text{per}}^\infty(\mathbb{R}^2), w(y_1, y_2, \cdot) \in C_0^\infty(\mathbb{R}), w|_\Gamma = 0, \text{div } w = 0 \right\}.$$

Take the  $\mathbb{R}^3$ -scalar-product of  $w \in \mathcal{X}$  with the first equation of (5.10), integrate over  $Q_I$  and integrate by parts. The pressure term vanishes due to  $\text{div } w = 0$  for  $w \in \mathcal{X}$ , and the property  $\text{div } z = 0$  implies the identity  $\Delta z = \text{div}(e(z))$ . It results in

$$\int_{Q_I} 2\eta e(z) : e(w) \, dy = - \int_{Q_I} (2\eta e(u) : e(w) + \eta \Delta \tilde{v} \cdot w) \, dy.$$

Let  $X$  be the closure of  $\mathcal{X}$  with respect to the norm

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

which indeed is a norm on  $\mathcal{X}$  due the condition  $w|_\Gamma = 0$ .  $X$  is a Hilbert space. A **weak formulation of the problem** (5.10), (5.11) is given by

**Problem 5.3.** Find  $z \in X$  such that

$$a(z, w) = \ell(w), \quad \text{for all } w \in X, \quad (5.12)$$

where

$$a(z, w) := \int_{Q_I} 2\eta e(z) : e(w) \, dy, \quad \ell(w) := - \int_{Q_I} (2\eta e(u) : e(w) + \eta \Delta \tilde{v} \cdot w) \, dy.$$

Note, that Poincaré's and the Second Korn inequality are in general not valid for unbounded domains as  $Q_I$ . Therefore, the bilinear form  $a$  might not be  $H^1$ -elliptic and  $X$  not equal to the closure of  $\mathcal{X}$  with respect to the  $H^1$ -norm.

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

**Theorem 5.4** (Existence and uniqueness of a weak solution of the Stokes problem). *For any fixed time  $t \in I$  and any point  $x \in S_0$ , problem 5.3 has a unique solution  $z(x, t) \in X$ . Furthermore, there exists a function  $p(x, t) \in L_{2,\text{loc}}(Q_I)$  with  $\lim_{y_3 \rightarrow \infty} p = P$  such that*

$$-\eta \Delta z + \nabla p = \eta(\Delta u + \Delta \tilde{v})$$

*in the distributional sense in  $Q_I$ . Concerning the semi-infinite domain  $Q_I$ ,  $z$  satisfies the estimate*

$$\|z(x, t)\|_X \leq c_1(\kappa) (|C^\nu(x, t)| + \|c_s(x, t)\|_{H^{1/2}(Y)}) + c_2 |\nabla V(x, t)|, \quad (5.13)$$

*with  $\kappa$  from (5.1). Restricting all functions to the bounded subdomain  $Q_{I\kappa} \subset Q_I$ , it is*

$$\begin{aligned} & \|v(x, t)\|_{H^1(Q_{I\kappa})} + \|p(x, t)\|_{L_2(Q_{I\kappa})} \\ & \leq c_3(\kappa) (|C^\nu(x, t)| + \|c_s(x, t)\|_{H^{1/2}(Y)}) + c_4 (|\nabla V(x, t)| + |P(x, t)|). \end{aligned} \quad (5.14)$$

The proof of this theorem needs the following version of the First Korn inequality:

**Proposition 5.5.** *Suppose  $\Omega = Y \times \mathbb{R}$  with  $Y = [0, 1]^2$  and set*

$$\mathcal{W} = \{w|_\Omega \mid w(\cdot, \cdot, y_3) \in C_{\text{per}}^\infty(\mathbb{R}^2), w(y_1, y_2, \cdot) \in C_0^\infty(\mathbb{R}), w(y_1, y_2, 0) = 0\}.$$

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

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

*Proof.* The proof uses ideas from [29], Chapter 2.5, Lemma 5.2. Let  $\hat{u}$  be the Fourier transform of  $u$  with respect to  $y_3$ ,

$$\hat{u}(y_1, y_2, \xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} u(y_1, y_2, y_3) e^{-i\xi y_3} dy_3.$$

The Fourier transform is a unitary transform,

$$\int_{\mathbb{R}} u(y_1, y_2, y_3) \overline{v(y_1, y_2, y_3)} dy_3 = \int_{\mathbb{R}} \hat{u}(y_1, y_2, \xi) \overline{\hat{v}(y_1, y_2, \xi)} d\xi$$

and in particular

$$\int_{\mathbb{R}} |u(y_1, y_2, y_3)|^2 dy_3 = \int_{\mathbb{R}} |\hat{u}(y_1, y_2, \xi)|^2 d\xi$$

holds. Expand  $\hat{u}$  into a Fourier series with respect to  $y_1$  and  $y_2$ : For  $k = 1, 2, 3$  it is

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

with coefficients  $c_{kmn}$  given by

$$c_{kmn} = \int_Y \hat{u}_k(y_1, y_2, \xi) e^{-2\pi i(m y_1 + n y_2)} dy_1 dy_2.$$

Parseval's equality yields

$$\int_Y |\hat{u}_k(y_1, y_2, \xi)|^2 dy_1 dy_2 = \sum_{m, n=-\infty}^{\infty} |c_{kmn}|^2.$$

From this representation follows

$$\begin{aligned} \|e(u)\|_{L_2(\Omega)}^2 &= \int_{\Omega} \left[ (\partial_1 u_1)^2 + (\partial_2 u_2)^2 + (\partial_3 u_3)^2 \right. \\ &\quad \left. + \frac{1}{2}(\partial_1 u_2 + \partial_2 u_1)^2 + \frac{1}{2}(\partial_1 u_3 + \partial_3 u_1)^2 + \frac{1}{2}(\partial_3 u_2 + \partial_2 u_3)^2 \right] dy \\ &= \int_{\mathbb{R}} \sum_{m, n=-\infty}^{\infty} \left[ 4\pi^2 m^2 |c_{1mn}|^2 + 4\pi^2 n^2 |c_{2mn}|^2 + \xi^2 |c_{3mn}|^2 \right. \\ &\quad \left. + 2\pi^2 m^2 |c_{2mn}|^2 + 2\pi^2 n^2 |c_{1mn}|^2 + 2\pi^2 m^2 |c_{3mn}|^2 + 2\pi^2 n^2 |c_{3mn}|^2 \right. \\ &\quad \left. + \frac{1}{2}\xi^2 |c_{1mn}|^2 + \frac{1}{2}\xi^2 |c_{2mn}|^2 + 4\pi^2 mn \operatorname{Re}(c_{1mn} \overline{c_{2mn}}) \right. \\ &\quad \left. + 2\pi m \operatorname{Re}(i\xi c_{1mn} \overline{c_{3mn}}) + 2\pi n \operatorname{Re}(i\xi c_{2mn} \overline{c_{3mn}}) \right] d\xi \\ &= \frac{1}{2} \|\nabla u\|_{L_2(\Omega)}^2 + \int_{\mathbb{R}} \sum_{m, n=-\infty}^{\infty} \left[ 2\pi^2 m^2 |c_{1mn}|^2 + 2\pi^2 n^2 |c_{2mn}|^2 \right. \\ &\quad \left. + \frac{1}{2}\xi^2 |c_{3mn}|^2 + 4\pi^2 mn \operatorname{Re}(c_{1mn} \overline{c_{2mn}}) + 2\pi m \operatorname{Re}(i\xi c_{1mn} \overline{c_{3mn}}) \right. \\ &\quad \left. + 2\pi n \operatorname{Re}(i\xi c_{2mn} \overline{c_{3mn}}) \right] d\xi \\ &\geq \frac{1}{2} \|\nabla u\|_{L_2(\Omega)}^2, \end{aligned}$$

since

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

with  $z_1 = 2\pi m c_{1mn}$ ,  $z_2 = 2\pi n c_{2mn}$ ,  $z_3 = i\xi c_{3mn}$ . Note, that the order of differentiation and the infinite sum of the Fourier series is changed in the above calculations. This can be done for continuously differentiable  $Y$ -periodic functions, see e.g. [34], chapter 2.4. Since these functions are dense in the space  $W$ , the result can be extended to  $W$ .  $\square$

*Proof of theorem 5.4. Existence of  $z$ :*

Young's inequality implies

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

for all  $z \in X$ . This yields the continuity of  $a$ :

$$|a(z, w)| \leq 2\eta \|e(z)\|_{L_2(Q_I)} \|e(w)\|_{L_2(Q_I)} \leq 2\eta \|z\|_X \|w\|_X.$$

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

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

The extended function  $z$  belongs to the space  $W$  defined in Proposition 5.5 and therefore

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

Hence  $a$  is  $X$ -elliptic and due to the Lax-Milgram Theorem, there is a unique solution  $z$  of problem 5.3 which satisfies

$$\|z\|_X \leq c\|\ell\|_{X'}. \quad (5.15)$$

**Existence of  $p$ :**

For the solution  $z$  of problem 5.3 the mapping  $a(z, \cdot) - \ell(\cdot)$  belongs to the space  $[H^{-1}(Q_I)]^3$  with

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

Since  $\{\nu \in [C_0^\infty(Q_I)]^3 \mid \operatorname{div} \nu = 0\} \subset \mathcal{X}$  holds, Propositions 1.1 and 1.2 in [52], Ch.1, §1, pp. 14-15, imply that there exists a function  $p \in L_{2,\text{loc}}(Q_I)$ , uniquely defined up to a constant, such that

$$-\eta \Delta z + \nabla p = \eta (\Delta u + \Delta \tilde{v})$$

in the distributional sense in  $Q_I$  with

$$\|\nabla p\|_{H^{-1}(Q_I)} \leq c (\|\nabla z\|_{L_2(Q_I)} + \|\nabla u + \Delta \tilde{v}\|_{L_2(Q_I)}). \quad (5.16)$$

It remains to prove that this constant can be chosen in such a way that

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

Therefore, it suffices to show that  $p$  becomes constant if  $y_3$  tends to infinity. Define for  $N \in \mathbb{N}$  and  $w \in [H_0^1(Q_I)]^3$

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

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

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

and thus

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

The last expression tends to zero for  $N \rightarrow \infty$  since  $\|\nabla z\|_{L_2(Q_I)} < \infty$ . It follows that  $\nabla p \rightarrow 0$  in  $H^{-1}(\Omega_N)$  which implies, together with VI. Satz in [55], p.88, that  $p$  becomes constant if  $y_3$  tends to infinity.

**Estimate for the right hand side:**

It is proven in Lemma 5.2 that

$$\|\nabla u\|_{L_2(Q_I)} \leq c (1 + \|\phi\|_{C^2(Y)})^3 \|v_\Gamma - \bar{v}\|_{H^{1/2}(Y)}.$$

Furthermore it follows from the definition of  $v_\Gamma$ , see (3.34), that

$$\|\bar{v}\|_{H^{1/2}(Y)} = \frac{\int_\Gamma v_\Gamma \cdot n \, ds}{\int_\Gamma n_3 \, ds} \|1\|_{L_2(Y)} \leq c(\kappa) (|C^\nu| + \|c_s\|_{L_2(Y)})$$

and

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

The definitions of  $\ell$  and  $\tilde{v}$  imply

$$\|\ell\|_{X'} \leq c \|\nabla u + \Delta \tilde{v}\|_{L_2(Q_I)} \leq c_1(\kappa) (|C^\nu| + \|c_s\|_{H^{1/2}(Y)}) + c_2 |\nabla V|.$$

In combination with (5.15), this proves (5.13).

**Restriction to  $Q_{IK}$ :**

For the velocity it follows from (5.13), Poincaré's inequality for  $z$  in  $Q_{IK}$ , and the definition of  $\tilde{v}$  and  $\bar{v}$

$$\|v\|_{H^1(Q_{IK})} \leq \|z + u + \bar{v} + \tilde{v}\|_{H^1(Q_{IK})} \leq c_1(\kappa) (|C^\nu| + \|c_s\|_{H^{1/2}(Y)}) + c_2 |\nabla V|.$$

The pressure can be estimated in the following way: For its gradient, estimates (5.16) and (5.13), Lemma 5.2 and the definition of  $\tilde{v}$  imply

$$\|\nabla p\|_{H^{-1}(Q_I)} \leq c_1(\kappa) (|C^\nu| + \|c_s\|_{H^{1/2}(Y)}) + c_2 |\nabla V|. \quad (5.17)$$

In order to estimate  $\|p\|_{L_2(Q_{IK})}$ , consider first for  $K \leq R < \infty$  the bounded domain  $Q_{IK} \subset Q_{IR} \subset Q_I$ . It follows from Proposition 1.2 in [52], Ch. I, §1, pp.14-15, that  $p \in L_2(Q_{IR})$ . With the transformation  $\Psi_I$ , see (5.3), define  $\hat{p} = p \circ \Psi_I \in L_2(\hat{Q}_{IR})$ . It is  $\nabla \hat{p} \in [H^{-1}(\hat{Q}_{IR})]^3$  with

$$\|\nabla \hat{p}\|_{H^{-1}(\hat{Q}_{IR})} \leq c (1 + \|D\phi\|_{L_\infty(Y)}) \|\nabla p\|_{H^{-1}(Q_{IR})} \leq c (1 + \|D\phi\|_{L_\infty(Y)}) \|\nabla p\|_{H^{-1}(Q_I)}.$$

It follows again from Proposition 1.2 in [52], Ch. I, §1, pp.14-15:

$$\begin{aligned} \|p\|_{L_2(Q_{IR})/\mathbb{R}} &= \|\hat{p}\|_{L_2(\hat{Q}_{IR})/\mathbb{R}} \\ &\leq c \|\nabla \hat{p}\|_{H^{-1}(\hat{Q}_{IR})} \\ &\leq c (1 + \|D\phi\|_{L_\infty(Y)}) \|\nabla p\|_{H^{-1}(Q_{IR})} \\ &\leq c (1 + \|D\phi\|_{L_\infty(Y)}) \|\nabla p\|_{H^{-1}(Q_I)}. \end{aligned} \quad (5.18)$$

Note, that the last term on the right-hand side is independent of  $R$ . Split  $p$  now additively in the following way:

$$p = p_0 + p_1 + P,$$

with  $\int_{Q_{IR}} p_0 \, dy = 0$  and a constant

$$p_1 = \frac{1}{R} \int_{Q_{IR}} (p - P) \, dy.$$

For  $p_0$  there holds

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

which can be estimated by (5.18). It remains to give an estimate for  $p_1$ : Note that  $\lim_{y_3 \rightarrow \infty} p = P$ , and therefore

$$\lim_{R \rightarrow \infty} \frac{1}{R} \int_{Q_{IR}} (p - P) \, dy = 0.$$

Choose now  $R > 0$  such that

$$|p_1| = \left| \frac{1}{R} \int_{Q_{IR}} (p - P) \, dy \right| \leq |C^\nu| + \|c_s\|_{H^{1/2}(Y)}. \quad (5.19)$$

It follows from (5.17), (5.18) and (5.19)

$$\begin{aligned} \|p\|_{L_2(Q_{IK})} &= \|p_0 + p_1 + P\|_{L_2(Q_{IK})} \\ &\leq \|p_0\|_{L_2(Q_{IR})} + |Q_{IK}|^{\frac{1}{2}} (p_1 + P) \\ &\leq c_1(\kappa) (|C^\nu| + \|c_s\|_{H^{1/2}(Y)}) + c_2 (|\nabla V| + |P|). \end{aligned}$$

This finishes the proof.  $\square$

Study now the regularity of the restrictions of  $v$  and  $p$  to  $Q_{IK}$  applying classical regularity results for the Stokes problem, namely Propositions 2.2 and 2.3 in [52], Ch.I, §2, pp.33-35. These results concern the Stokes equations with Dirichlet boundary conditions and can be used to prove the following theorem:

**Theorem 5.6** (Spatial regularity). *Suppose  $2 \leq r < \infty$ ,  $\phi \in C_{\text{per}}^2(Y)$  with  $\|\phi\|_{C^2(Y)} \leq \kappa$ , with  $\kappa$  from (5.1), and  $c_s \in W_{r,\text{per}}^{2-1/r}(Y)$ . Then, for fixed  $x \in S_0$ ,  $t \in I$ , the solution  $(v, p)(x, t)$  of the Stokes problem satisfies  $v \in [W_{r,\text{per}}^2(Q_{IK})]^3$ ,  $p \in W_{r,\text{per}}^1(Q_{IK})$ , and the a priori estimate*

$$\begin{aligned} &\|v(x, t)\|_{W_r^2(Q_{IK})} + \|p(x, t)\|_{W_r^1(Q_{IK})} \\ &\leq c(\kappa) \left( \|c_s(x, t)\|_{W_r^{2-1/r}(Y)} + |C^\nu(x, t)| + |\nabla V(x, t)| + |P(x, t)| \right). \end{aligned} \quad (5.20)$$

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

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

For  $\text{supp}(\chi_i) \cap \Gamma \neq \emptyset$  define  $\Omega_i := \{y \in \text{supp}(\chi_i) : y_3 > h_A \phi(y_1, y_2)\}$  (where  $\phi$  is extended periodically to  $\mathbb{R}^2$ ), and  $\Omega_i := \text{supp}(\chi_i)$  else. Note, that  $v$  and  $p$  can be interpreted as functions in  $\Omega_i$  after an eventual periodic extension to  $(y_1, y_2) \in \mathbb{R}^2$  or considering the solutions of Theorem 5.4 for  $y_3 > h_A \phi(y_1, y_2) + K$ . The functions  $\chi_i v$  and  $\chi_i p$  solve the local problem

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

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

Due to  $v \in [H^1(\Omega_i)]^3$ ,  $p \in L_2(\Omega_i)$ , a first application of Proposition 2.3 in [52], Ch.I, §2, p.35, implies that  $\chi_i v \in [W_r^1(\Omega_i)]^3$ ,  $\chi_i p \in L_r(\Omega_i)$  for  $2 \leq r \leq 6$ . Using this and applying the same result again gives  $\chi_i v \in [W_r^1(\Omega_i)]^3$ ,  $\chi_i p \in L_r(\Omega_i)$  for any  $r \geq 2$ . Employ the argument a third time to get  $\chi_i v \in [W_r^2(\Omega_i)]^3$ ,  $\chi_i p \in W_r^1(\Omega_i)$  for any  $r \geq 2$ , presuming  $c_s \in W_r^{2-1/r}(Y)$ . Proposition 2.3 in [52], Ch.I, §2, p.35, also implies an a priori estimate

$$\begin{aligned} &\|\chi_i v(x, t)\|_{W_r^2(\Omega_i)} + \|\chi_i p(x, t)\|_{W_r^1(\Omega_i)/\mathbb{R}} \\ &\leq c(\kappa) \left( \|c_s(x, t)\|_{W_r^{2-1/r}(Y)} + |C^y(x, t)| + |\nabla V(x, t)| \right), \end{aligned} \quad (5.21)$$

where the constant  $c$  depends on the corresponding domain. In particular, for some  $i \in \{1, \dots, M\}$ , this constant depends on  $\phi$ . In order to investigate this dependency, one has to go back to the  $L_r$ -estimates for elliptic problems by Agmon, Douglis and Nirenberg, see [2] and [3]. Use the transformation  $\Psi_i$  of Lemma 5.2 and consider the corresponding transformed local problems on  $\Psi_i^{-1}(\Omega_i)$ . The transformed systems of equations now have variable (and  $\phi$ -dependent) coefficients but still are uniformly elliptic in the sense of [3]. So, Theorem 10.5 of [3] can be applied. The constant in the estimate of Theorem 10.5 in [3] depends on a bound for the corresponding norms of the coefficients and the constant of uniform ellipticity, which can be estimated in terms of  $\kappa$  here, and is else independent of  $\phi$ . Then, Theorem 10.5 of [3] proves estimate (5.21). Due to

$$v = \sum_{i=1}^M \chi_i v, \quad p = \sum_{i=1}^M \chi_i p, \quad \text{a.e. in } Q_{IK},$$

it is

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

which proves (5.20).  $\square$

Study next the continuous dependency of  $v$  and  $p$  on the time  $t \in I$  and on the coupling data. Let  $C^{\mathcal{V}(1)}, C^{\mathcal{V}(2)}, V^{(1)}, V^{(2)}$  and  $P^{(1)}, P^{(2)}$  be two macroscopic volume concentrations, velocities and pressures,  $(\phi^{(1)}, c_s^{(1)}), (\phi^{(2)}, c_s^{(2)}) \in C_{\text{per}}^2(Y) \times W_{r,\text{per}}^{2-1/r}(Y)$  and  $(v^{(1)}, p^{(1)}), (v^{(2)}, p^{(2)})$  the corresponding solutions. Note that, if  $\phi^{(1)} \neq \phi^{(2)}$ , the domains of these two problems do not coincide. Therefore, transform both problems to the time independent domain  $\hat{Q}_I := Y \times (0, \infty)$  or  $\hat{Q}_{IK} = Y \times (0, K)$ , with the help of the transformations

$$\Psi_I^{(j)}(t) : \hat{Q}_I \rightarrow Q_I^{(j)}(t), \quad \text{or} \quad \Psi_{IK}^{(j)}(t) : \hat{Q}_{IK} \rightarrow Q_{IK}^{(j)}(t), \quad j = 1, 2,$$

defined in (5.3), and set be  $\hat{v}^{(j)} = v^{(j)} \circ \Psi_I^{(j)}, \hat{p}^{(j)} = p^{(j)} \circ \Psi_I^{(j)}, j = 1, 2$ . Then,  $\hat{v}^{(j)}, \hat{p}^{(j)}$  solve

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

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

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

with the Kronecker–delta  $\delta_{IK}$ , and

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

together with the boundary condition

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

A first step is the following result:

**Lemma 5.7.** *For fixed  $x \in S_0$  and  $t \in I$ , the solutions  $(v^{(j)}, p^{(j)})$ , which correspond to  $C^{\mathcal{V}(j)}, V^{(j)}, P^{(j)}$  and  $(\phi^{(j)}, c_s^{(j)}) \in C_{\text{per}}^2(Y) \times W_{r,\text{per}}^{2-1/r}(Y), j = 1, 2$ , satisfy*

$$\begin{aligned} & \|(\hat{v}^{(1)} - \hat{v}^{(2)})(x, t)\|_{W_r^2(Q_{IK})} + \|(\hat{p}^{(1)} - \hat{p}^{(2)})(x, t)\|_{W_r^1(Q_{IK})} \\ & \leq c(\kappa) \left( \| (c_s^{(1)} - c_s^{(2)})(x, t) \|_{W_r^{2-1/r}(Y)} + \| (\phi^{(1)} - \phi^{(2)})(x, t) \|_{C^2(Y)} \right. \\ & \quad + |(C^{\mathcal{V}(1)} - C^{\mathcal{V}(2)})(x, t)| + |(\nabla_x V^{(1)} - \nabla_x V^{(2)})(x, t)| \\ & \quad \left. + |(P^{(1)} - P^{(2)})(x, t)| \right) \end{aligned} \quad (5.22)$$

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

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

with

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

and

$$\begin{aligned} \lim_{\hat{y}_3 \rightarrow \infty} \left( \nabla_{\hat{y}}(\hat{v}^{(1)} - \hat{v}^{(2)}) + (\nabla_{\hat{y}}(\hat{v}^{(1)} - \hat{v}^{(2)}))^{\top} \right) e_3 \\ = \left( \nabla_x(V^{(1)} - V^{(2)}) + (\nabla_x(V^{(1)} - V^{(2)}))^{\top} \right) \Big|_{x_3=0} e_3, \end{aligned} \quad (5.23)$$

$$\lim_{\hat{y}_3 \rightarrow \infty} (\hat{p}^{(1)} - \hat{p}^{(2)}) = (P^{(1)} - P^{(2)}) \Big|_{x_3=0}, \quad (5.24)$$

Analogously to the proof of Theorem 5.6, it is

$$\begin{aligned} & \|\hat{v}^{(1)} - \hat{v}^{(2)}\|_{W_r^2(Q_{IK})} + \|\hat{p}^{(1)} - \hat{p}^{(2)}\|_{W_r^1(Q_{IK})/\mathbb{R}} \\ & \leq c(\kappa) \left( \|c_s^{(1)} - c_s^{(2)}\|_{W_r^{2-1/r}(\gamma)} + \|\phi^{(1)} - \phi^{(2)}\|_{C^2(\gamma)} + |C^{\nu(1)} - C^{\nu(2)}| \right. \\ & \quad \left. + |\nabla_x V^{(1)} - \nabla_x V^{(2)}| \right). \end{aligned} \quad (5.25)$$

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

$$\int_{Q_{IK}} p_0^{(j)} dy = 0, \quad p_1^{(j)} = \frac{1}{|Q_{IK}|} \int_{Q_{IK}} p^{(j)} dy = \text{constant}.$$

As in the proof of Theorem 5.4, it follows

$$\begin{aligned} \|\nabla(\hat{p}^{(1)} - \hat{p}^{(2)})\|_{H^{-1}(Q_I)} \leq c(\kappa) \left( \|c_s^{(1)} - c_s^{(2)}\|_{W_r^{2-1/r}(\gamma)} + |C^{\nu(1)} - C^{\nu(2)}| \right. \\ \left. + |\nabla_x V^{(1)} - \nabla_x V^{(2)}| \right), \end{aligned}$$

and together with (5.24), this yields

$$\begin{aligned} |\hat{p}_1^{(1)} - \hat{p}_1^{(2)}| \leq c(\kappa) \left( \|c_s^{(1)} - c_s^{(2)}\|_{W_r^{2-1/r}(\gamma)} + |C^{\nu(1)} - C^{\nu(2)}| \right. \\ \left. + |\nabla_x V^{(1)} - \nabla_x V^{(2)}| + |P^{(1)} - P^{(2)}| \right). \end{aligned} \quad (5.26)$$

A combination of (5.25) and (5.26) finishes the proof.  $\square$

Lemma 5.7 is the basis for the following two results: Continuity of  $\hat{v}$  and  $\hat{p}$  with respect to time and with respect to the coupling data.

**Theorem 5.8** (Regularity in space and time). *Suppose  $c_s \in C(I, W_{r,\text{per}}^{2-1/r}(Y))$  and  $\phi \in C(I, C_{\text{per}}^2(Y))$ . The solution  $(v, p)(t)$  of the Stokes problem (3.33), (3.34), (3.35) satisfies*

$$\hat{v} \in C(I, [W_{r,\text{per}}^2(\hat{Q}_{IK})]^3), \quad \hat{p} \in C(I, W_{r,\text{per}}^1(\hat{Q}_{IK})).$$

The estimate

$$\begin{aligned} & \|\hat{v}(x)\|_{C(I, W_r^2(\hat{Q}_{IK}))} + \|\hat{p}(x)\|_{C(I, W_r^1(\hat{Q}_{IK}))} \\ & \leq c(\kappa) \left( \|c_s(x)\|_{C(I, W_r^{2-1/r}(Y))} + \|C^{\mathcal{V}}(x)\|_{C(I)} + \|\nabla_x V(x)\|_{C(I)} + \|P(x)\|_{C(I)} \right) \end{aligned} \quad (5.27)$$

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

*Proof.* For  $t_j \in I$ ,  $j = 1, 2$ , replace  $f^{(j)} = f(t_j)$  for  $f \in \{v, p, C^{\mathcal{V}}, c_s, \phi, V, P\}$  in the proof of Lemma 5.7. Since  $C^{\mathcal{V}}, c_s, \phi, V, P$  are supposed to be continuous in time,  $\hat{v}$  and  $\hat{p}$  are continuous in time. Note, that

$$\|\hat{v}(x, t)\|_{W_r^2(\hat{Q}_{IK})} + \|\hat{p}(x, t)\|_{W_r^1(\hat{Q}_{IK})} \leq c(\kappa) (\|v(x, t)\|_{W_r^2(Q_{IK})} + \|p(x, t)\|_{W_r^1(Q_{IK})}).$$

Combination of this estimate with (5.20) and taking the maximum on  $t \in I$  proves (5.27).  $\square$

**Lemma 5.9** (Continuity with respect to the coupling data). *Suppose  $c_{s,i} \in C(I, W_{r,\text{per}}^{2-1/r}(Y))$ ,  $\phi_i \in C(I, C_{\text{per}}^2(Y))$  and  $C_i^{\mathcal{V}} \in C(I)$ ,  $i = 1, 2$ , and denote by  $v_i, p_i$  the corresponding solutions of the Stokes problem. Then, the estimate*

$$\begin{aligned} & \|(\hat{v}_1 - \hat{v}_2)(x)\|_{C(I, W_r^2(\hat{Q}_{IK}))} + \|(\hat{p}_1 - \hat{p}_2)(x)\|_{C(I, W_r^1(\hat{Q}_{IK}))} \\ & \leq c(\kappa) \left( \|(\phi_1 - \phi_2)(x)\|_{C(I, C^2(Y))} + \|(c_{s,1} - c_{s,2})(x)\|_{C(I, W_r^{2-1/r}(Y))} \right. \\ & \quad \left. + \|(C_1^{\mathcal{V}} - C_2^{\mathcal{V}})(x)\|_{C(I)} \right) \end{aligned}$$

holds true, where  $\kappa = \max\{\|\phi_1\|_{C(I, C^2(Y))}, \|\phi_2\|_{C(I, C^2(Y))}\}$ .

*Proof.* Take the maximum on  $t \in I$  in (5.22) with  $V^{(1)} = V^{(2)}$  and  $P^{(1)} = P^{(2)}$ .  $\square$

### 5.2.2 The Microscopic Elastic Equation

This section analyzes the elasticity problem (3.37), (3.38), (3.39). Suppose in the following that  $\hat{v} \in C(I, [W_{r,\text{per}}^2(\hat{Q}_{IK})]^3)$ ,  $\hat{p} \in C(I, W_{r,\text{per}}^1(\hat{Q}_{IK}))$  and  $\phi \in C(I, C_{\text{per}}^2(Y))$  with  $\phi(t, y) > 0$  for all  $(t, y) \in I \times \bar{Y}$ . Analogously to section 5.2.1, a transformation  $\Psi_s$  of  $Q_s$  into a time independent domain  $\hat{Q}_s$  is used in the coming proofs. The displacement field on the transformed domain is denoted by  $\hat{u} = u \circ \Psi_s$ . The basic idea for the transformation is the same as for the definition of  $\Psi_I$  in (5.3), the construction of  $\Psi_s$  works out as follows:

Denote by  $R = h_A \max_{t \in I, y \in Y} |\phi(t, y)|$  a time independent upper bound for the thickness of  $Q_s(t)$  in  $y_3$ -direction and define  $\hat{Q}_s = Y \times [0, R]$  and the transformation

$$\Psi_s(t) : \hat{Q}_s \rightarrow \tilde{Q}_s(t) : (\hat{y}_1, \hat{y}_2, \hat{y}_3)^\top \mapsto (\hat{y}_1, \hat{y}_2, \hat{y}_3 + h_A \phi(t, y_1, y_2) - R)^\top, \quad (5.28)$$

(compare the transformation (5.3)), where  $\tilde{Q}_s$  is the range of  $\hat{Q}_s$  under  $\Psi_s$ . Note, that  $\tilde{Q}_s$  is in general a strict superset of  $Q_s$ , and therefore, the function  $\hat{u} = u \circ \Psi_s$  is not well-defined, if  $u$  is only defined on  $Q_s$ . But any function  $u \in W_{r,\text{per}}^2(Q_s)$  can be extended to  $W_{r,\text{per}}^2(\tilde{Q}_s)$  in such a way that

$$\|u\|_{W_r^2(Q_s)} \leq \|u\|_{W_r^2(\tilde{Q}_s)} \leq c \|u\|_{W_r^2(Q_s)},$$

with a constant  $c$  depending only on  $r$ , thanks to Theorem 5.19 in [1], p.148. Therefore, the following does not distinguish between  $u$  defined on  $\tilde{Q}_s$  and  $Q_s$ .

For the boundary condition  $u = b$  on  $\tilde{\Gamma}$ , it is assumed throughout this section that  $b$  is the trace of a function  $\bar{u} \in [W_{r,\text{per}}^2(Q_s)]^3$ , with

$$\|\bar{u}\|_{W_{r,\text{per}}^2(Q_s)} \leq c \|b\|_{W_r^{2-1/r}(\tilde{\Gamma})},$$

for some  $2 \leq r < \infty$ . Inserting  $z = u - \bar{u}$  in (3.37), (3.38), (3.39) leads to

$$\begin{aligned} -\operatorname{div} \sigma(z) &= \operatorname{div} \sigma(\bar{u}) && \text{in } Q_s, \\ \sigma(z)n &= g - \sigma(\bar{u})n && \text{on } \Gamma, \\ z &= 0 && \text{on } \tilde{\Gamma}, \\ z &\text{ is } Y\text{-periodic,} \end{aligned} \quad (5.29)$$

where  $g = 2\eta e(v)n - pn$ . In order to derive a weak formulation of the problem, assume for the moment that all functions are smooth. Let  $w$  be  $Y$ -periodic with  $w|_{\tilde{\Gamma}} = 0$ . Take the  $\mathbb{R}^3$ -scalar product of (5.29) with  $w$ , integrate over  $Q_s$ , integrate by parts and get due to the boundary conditions :

$$\int_{Q_s} \sigma(z) : e(w) \, dy = - \int_{Q_s} \sigma(\bar{u}) : e(w) \, dy + \int_{\Gamma} g \cdot w \, ds.$$

Denote

$$a(z, w) := \int_{Q_s} \sigma(z) : e(w) \, dy, \quad \ell(w) := - \int_{Q_s} \sigma(\bar{u}) : e(w) \, dy + \int_{\Gamma} g \cdot w \, ds.$$

Introduce the space

$$X = \{v \in [H_{\text{per}}^1(Q_s)]^3 \mid v|_{\bar{\Gamma}} = 0\}$$

and state the **weak formulation of the problem** (5.29):

**Problem 5.10.** Find  $z \in X$  such that

$$a(z, w) = \ell(w), \quad \text{for all } w \in X. \quad (5.30)$$

In order to prove  $X$ -ellipticity of the bilinear form  $a$ , the following version of Korn's inequality is needed:

**Proposition 5.11.** Let  $Y = [0, 1]^2$ . Every  $z \in X$  satisfies

$$\int_{Q_s} e(z) : e(z) \, dy \geq \frac{c}{(1 + \|\phi\|_{L_\infty(Y)})^2 (1 + \|D\phi\|_{L_\infty(Y)})^4} \|z\|_{H^1(Q_s)}^2, \quad (5.31)$$

where the constant  $c$  is independent of  $\phi$ .

*Proof.* Let  $z \in X$ . Extend  $z$  by zero for  $y_3 < 0$  and set  $\hat{y} = \Psi_s^{-1}(y)$ . It is

$$\begin{aligned} \|\nabla_y z\|_{L_2(Q_s)} &\leq C (1 + \|D\phi\|_{L_\infty(Y)}) \|\nabla_{\hat{y}}(z \circ \Psi_s)\|_{L_2(\hat{Q}_s)}, \\ \|e_y(z \circ \Psi_s)\|_{L_2(\hat{Q}_s)} &\leq C (1 + \|D\phi\|_{L_\infty(Y)}) \|e_y(z)\|_{L_2(Q_s)}. \end{aligned}$$

Denote  $\hat{z} = z \circ \Psi_s$ . For  $\hat{z}$  the First Korn inequality on  $\hat{Q}_s$ , i.e.

$$\|\nabla_{\hat{y}} \hat{z}\|_{L_2(\hat{Q}_s)}^2 \leq 2 \|e_{\hat{y}}(\hat{z})\|_{L_2(\hat{Q}_s)}^2,$$

is proven by a combination of the proofs of [29], Chapter 2.5, Lemma 5.2 and Proposition 5.5. Consequently

$$\|\nabla_y z\|_{L_2(Q_s)} \leq c (1 + \|D\phi\|_{L_\infty(Y)})^2 \|e_y(z)\|_{L_2(Q_s)}, \quad (5.32)$$

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

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

□

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

**Theorem 5.12** (Existence and uniqueness of a weak solution of the elastic problem). For fixed  $x \in S_0$ ,  $t \in I$ , problem 5.10 has a unique solution  $z \in X$ .

*Proof.* The bilinear form  $a$  is  $X$ -elliptic due to Proposition 5.11 and continuous due to Young's and Cauchy-Schwarz' inequality. The right-hand side  $\ell$  belongs to  $X'$ , in fact it is  $g = 2\eta e(v)n - pn \in H^{1/2}(\Gamma)$  and  $\sigma(\bar{u}) \in H^1(Q_s)$ . The Lax-Milgram Theorem yields the result.  $\square$

Study further regularity properties of  $u$ , starting with spatial regularity:

**Theorem 5.13** (Spatial regularity). *Suppose that  $\|\phi\|_{C^2(Y)} < \kappa$ , for a constant  $\kappa > 0$ , and  $b \in [W_r^{2-1/r}(\tilde{\Gamma})]^3$  is the trace of a function  $\bar{u} \in [W_{r,\text{per}}^2(Q_s)]^3$ . Then, the weak solution  $z$  is an element of  $[W_{r,\text{per}}^2(Q_s)]^3$  and the displacement field  $u = z + \bar{u}$  satisfies the a priori estimate*

$$\begin{aligned} & \|u(x, t)\|_{W_r^2(Q_s)} \\ & \leq c(\kappa) \left( \|v(x, t)\|_{W_r^2(Q_{IK})} + \|\rho(x, t)\|_{W_r^1(Q_{IK})} + \|b(x, t)\|_{W_r^{2-1/r}(\tilde{\Gamma})} \right). \end{aligned} \quad (5.33)$$

*Proof.* Proceed as in the proof of Theorem 5.6 and localize the problem using a partition of unity  $(\chi_i)_{i=1,\dots,M}$ . If  $\text{supp}(\chi_i) \cap \Gamma = \emptyset$ , then it follows from the classical regularity results for the linear elastic problem with Dirichlet boundary conditions (see e.g. [53], Ch.III, §7, p.80, Theorem 7.1) that  $\chi_i z \in [W_r^2(\Omega_i)]^3$ . For  $\text{supp}(\chi_i) \cap \Gamma \neq \emptyset$ , the same conclusion can be made using the corresponding results for Neumann boundary conditions (see e.g. [53], Ch.III, §7, p.83, Lemma 7.5). Analogously to the proof of Theorem 5.6, the estimate (5.33) can be derived using the  $L_r$ -estimates of Agmon, Douglis, Nirenberg (see [2], [3]) after a local transformation of the problems to domains with  $\phi$ -independent boundary, but  $\phi$ -dependent coefficients. In addition to the arguments of Theorem 5.6, note the following fact: After applying Theorem 10.5 of [3] to the localized and transformed elastic problems, the constant in the resulting estimate also depends on the constant of Korn's inequality. Thanks to Proposition 5.11, this constant can also be estimated in terms of  $\kappa$ .  $\square$

**Theorem 5.14** (Regularity in space and time). *Suppose  $\phi \in C(I, C_{\text{per}}^2(Y))$  with  $\phi(t, y) > 0$  for all  $(t, y) \in I \times \bar{Y}$ , and  $\hat{v} \in C(I, [W_{r,\text{per}}^2(\hat{Q}_{IK})]^3)$ ,  $\hat{p} \in C(I, W_{r,\text{per}}^1(\hat{Q}_{IK}))$ . The solution  $u(t)$  of the elastic problem (3.37), (3.38), (3.39) satisfies*

$$\hat{u} \in C(I, W_{r,\text{per}}^2(\hat{Q}_s)),$$

and

$$\begin{aligned} \|\hat{u}(x)\|_{C(I, W_r^2(\hat{Q}_s))} & \leq c(\kappa) \left( \|\hat{v}(x)\|_{C(I, W_r^2(\hat{Q}_{IK}))} + \|\hat{p}(x)\|_{C(I, W_r^1(\hat{Q}_{IK}))} \right. \\ & \quad \left. + \|b(x)\|_{C(I, W_r^{2-1/r}(\tilde{\Gamma}))} \right), \end{aligned} \quad (5.34)$$

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

*Proof.* The continuity of  $\hat{u}$  with respect to  $t$  follows as in the proof of Lemma 5.7 and Theorem 5.8. Estimate (5.34) follows from

$$\begin{aligned} & \|\hat{u}(x, t)\|_{W_r^2(\hat{Q}_s)} \leq c(\kappa) \|u(x, t)\|_{W_r^2(Q_s)}, \\ & \|v(x, t)\|_{W_r^2(Q_{IK})} + \|\rho(x, t)\|_{W_r^1(Q_{IK})} \leq c(\kappa) \left( \|\hat{v}(x, t)\|_{W_r^2(\hat{Q}_{IK})} + \|\hat{p}(x, t)\|_{W_r^1(\hat{Q}_{IK})} \right), \end{aligned}$$

by taking the maximum on  $t \in I$  in (5.33).  $\square$

**Lemma 5.15** (Continuity with respect to the coupling data). *Suppose  $\phi_i \in C(I, C_{\text{per}}^2(Y))$  with  $\phi(t, y) > 0$  for all  $(t, y) \in I \times \bar{Y}$ , and  $\hat{v}_i \in C(I, [W_{r, \text{per}}^2(\hat{Q}_{I\kappa})]^3)$ ,  $\hat{p}_i \in C(I, W_{r, \text{per}}^1(\hat{Q}_{I\kappa}))$ ,  $i = 1, 2$ , and denote by  $u_i$  the corresponding solutions of the elastic problem. Then, the estimate*

$$\begin{aligned} \|(\hat{u}_1 - \hat{u}_2)(x)\|_{C(I, W_r^2(\hat{Q}_{I\kappa}))} &\leq c(\kappa) \left( \|(\hat{v}_1 - \hat{v}_2)(x)\|_{C(I, W_r^2(\hat{Q}_{I\kappa}))} \right. \\ &\quad + \|(\hat{p}_1 - \hat{p}_2)(x)\|_{C(I, W_r^1(\hat{Q}_{I\kappa}))} \\ &\quad \left. + \|(\phi_1 - \phi_2)(x)\|_{C(I, C^2(Y))} \right), \end{aligned}$$

holds true, where  $\kappa = \max\{\|\phi_1\|_{C(I, C^2(Y))}, \|\phi_2\|_{C(I, C^2(Y))}\}$ .

*Proof.* The statement follows as in the proof of Lemma 5.9.  $\square$

### 5.2.3 The Microscopic Phase Field Model

This section discusses the solvability of the phase field version of the microscopic BCF-model (3.40) and (3.41) with initial conditions (3.42)

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

and periodic boundary conditions with respect to  $(y_1, y_2) \in Y$ . This system has to be solved for the phase field  $\phi$  and the surface concentration  $c_s$ . These equations are posed for every  $x \in S_0$  in  $I \times Y$ , where  $I = [0, T]$  is a time interval and  $Y$  a twodimensional periodicity cell.

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 (3.43). The second is  $\kappa$  from (5.1), which does not occur explicitly in the equations, but implicitly through  $u$ . Here,  $\kappa$  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 (3.43) has to be understood in the trace sense. As explained in the beginning of section 5.1, 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  $C(I, [W_{r,per}^2(\hat{Q}_s)]^3)$ . 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 (3.43) as

$$q(\phi, c_s, u) = \frac{\xi RT \rho_s}{c_{eq} \gamma \beta} (c_{eq} - c_s) g(\phi) + \frac{\xi h_A \rho_s}{2 c_{eq} \gamma \beta} \sigma(u) : e(u).$$

For  $u$  and  $\hat{u}$  there is the pointwise relation

$$c_1(\kappa) |e(\hat{u})(t, y)| \leq |e(u)(t, y)| \leq c_2(\kappa) |e(\hat{u})(t, y)|, \quad t \in I \text{ and a.e. in } Y, \quad (5.35)$$

and the relation for the norms

$$c_1(\kappa) \|\hat{u}(t)\|_{W_r^2(\hat{Q}_s)} \leq \|u(t)\|_{W_r^2(Q_s(t))} \leq c_2(\kappa) \|\hat{u}(t)\|_{W_r^2(\hat{Q}_s)}, \quad t \in I, \quad (5.36)$$

with  $\kappa$  from (5.1). ( $\kappa$  occurs when calculating derivatives of  $u \circ \Psi_s$  and  $\hat{u} \circ \Psi_s^{-1}$ , where the chain rule has to be applied.  $\kappa$  is a bound for the derivatives of  $\Psi_s$  and  $\Psi_s^{-1}$ , compare also section 5.2.2.)

The functions  $f'$  and  $\hat{q}$  have the following properties:

**Proposition 5.16.** *Suppose  $f(\phi) = -\cos(2\pi\phi)$  and  $q$  is given by (3.43). Then  $f'$  and  $\hat{q}$  satisfy the growth condition*

$$|f'(\phi)| + |\hat{q}(\phi, c_s, \hat{u})| \leq c(\kappa) (1 + |\nabla \hat{u}|^2 + |c_s| + |\phi|), \quad (5.37)$$

and the Lipschitz condition

$$\begin{aligned} & |f'(\phi_1) - f'(\phi_2)| + |\hat{q}(\phi_1, c_{s,1}, \hat{u}_1) - \hat{q}(\phi_2, c_{s,2}, \hat{u}_2)| \\ & \leq c(\kappa) (|\phi_1 - \phi_2| + |c_{s,1} - c_{s,2}| + |\nabla(\hat{u}_1 + \hat{u}_2)| |\nabla(\hat{u}_1 - \hat{u}_2)|). \end{aligned} \quad (5.38)$$

*Proof.* The growth condition follows directly from the definition of  $f$  and  $q$  and (5.35).  $f'$  and  $\hat{q}$  are Lipschitz continuous with respect to  $\phi$  and  $c_s$ , and due to (5.35) it is

$$\begin{aligned} & |f'(\phi_1) - f'(\phi_2)| + |\hat{q}(\phi_1, c_{s,1}, \hat{u}_1) - \hat{q}(\phi_2, c_{s,2}, \hat{u}_2)| \\ & \leq c(\kappa) (|\phi_1 - \phi_2| + |c_{s,1} - c_{s,2}| + |e(\hat{u}_1) : e(\hat{u}_1) - e(\hat{u}_2) : e(\hat{u}_2)|), \end{aligned}$$

where  $c > 0$  is independent of  $\phi_i, c_{s,i}$  and  $u_i$ , but depends, as the constant in (5.37), on  $\kappa$ . Furthermore, it is due to the third binomial formula

$$\begin{aligned} |e(\hat{u}_1) : e(\hat{u}_1) - e(\hat{u}_2) : e(\hat{u}_2)| &= |(e(\hat{u}_1) + e(\hat{u}_2)) : (e(\hat{u}_1) - e(\hat{u}_2))| \\ &= |e(\hat{u}_1 + \hat{u}_2) : e(\hat{u}_1 - \hat{u}_2)| \\ &\leq |\nabla(\hat{u}_1 + \hat{u}_2)| |\nabla(\hat{u}_1 - \hat{u}_2)|. \end{aligned}$$

Consequently,  $\hat{q}$  is at least locally Lipschitz continuous with respect to  $\hat{u}$  and (5.38) follows.  $\square$

In fact, the following proofs only use the abstract conditions (5.37) and (5.38) and not the exact definitions of  $f$  and  $q$ . Thus, all of the following results hold for any functions  $f$  and  $q$ , which satisfy (5.37) and (5.38).

Consider test functions  $w_1, w_2 \in L_2(I; H_{\text{per}}^1(Y))$ , multiply equations (3.40) and (3.41) with  $w_1$  and  $w_2$  respectively, integrate by parts and get the following **weak formulation**:

**Problem 5.17.** *Find  $c_s, \phi \in L_2(I; H_{\text{per}}^1(Y))$  with  $\partial_t c_s, \partial_t \phi \in L_2(I; H_{\text{per}}^1(Y)')$  such that the initial conditions (3.42) are satisfied and for every  $w_1, w_2 \in L_2(I; H_{\text{per}}^1(Y))$  the following equations hold true:*

$$\int_I \left( \tau \xi^2 \langle \partial_t \phi, w_1 \rangle + \int_Y (\xi^2 \nabla \phi \cdot \nabla w_1 + (f'(\phi) + \hat{q}(\phi, c_s, \hat{u})) w_1) dy \right) dt = 0. \quad (5.39)$$

$$\begin{aligned} & \int_I \left( \langle \partial_t c_s, w_2 \rangle + \varrho_s \langle \partial_t \phi, w_2 \rangle \right. \\ & \quad \left. + \int_Y \left( D_s \nabla c_s \cdot \nabla w_2 + \left( \frac{c_s}{\tau_s} - \frac{C^{\mathcal{V}}}{\tau^{\mathcal{V}}} \right) w_2 \right) dy \right) dt = 0, \end{aligned} \quad (5.40)$$

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

**Theorem 5.18** (Existence and uniqueness of a weak solution of the phase field model). Assume  $c_{s,ini} \in L_2(Y)$ ,  $\phi_{ini} \in L_2(Y)$  and  $\hat{u} \in L_2(I, [W_{r,per}^2(\hat{Q}_s)]^3)$ , for some  $r \geq 3$ . Furthermore, suppose that the constants  $D_s$ ,  $\tau$ ,  $\xi$ ,  $h_A$ ,  $\varrho_s$ ,  $\tau^\nu$  and  $\tau_s$  are positive. Then, the microscopic problem 5.17 at any fixed point  $x \in S_0$  with given  $C^\nu = C^\nu(\cdot, x) \in L_2(I)$  has a unique solution  $(\phi, c_s)$ . It satisfies

$$\begin{aligned} & \|\phi(x)\|_{L_\infty(I, L_2(Y))} + \|\phi(x)\|_{L_2(I, H^1(Y))} + \|c_s(x)\|_{L_\infty(I, L_2(Y))} + \|c_s(x)\|_{L_2(I, H^1(Y))} \\ & \leq c(\kappa) \left( 1 + \|\hat{u}(x)\|_{L_2(I, W_r^2(\hat{Q}_s))}^2 + \|C^\nu(x)\|_{L_2(I)} \right. \\ & \quad \left. + \|c_{s,ini}(x)\|_{L_2(Y)} + \|\phi_{ini}(x)\|_{L_2(Y)} \right), \end{aligned} \quad (5.41)$$

with  $\kappa$  from (5.1).

*Proof.* Investigate first the regularity of the coupling term. Due to the growth condition (5.37), the crucial coupling term to study is  $|\nabla \hat{u}|^2$ , which has to be understood in the trace sense as explained above. Suppose  $\hat{u} \in [W_{r,per}^2(\hat{Q}_s)]^3$ , for fixed  $t$ , then :

$$\begin{aligned} \hat{u} \in [W_r^2(\hat{Q}_s)]^3 & \Rightarrow |\nabla \hat{u}|^2 \in W_{r/2}^1(\hat{Q}_s) \\ & \Rightarrow \text{tr} |\nabla \hat{u}|^2 \in W_{r/2}^{1-2/r}(Y) \\ & \Rightarrow \text{tr} |\nabla \hat{u}|^2 \in L_2(Y), \quad \text{if } r \geq 3. \end{aligned}$$

For the norms there holds

$$\begin{aligned} \|\nabla \hat{u}\|_{L_2(Y)} & \leq c \|\nabla \hat{u}\|_{W_{r/2}^{1-2/r}(Y)} \leq c \|\nabla \hat{u}\|_{W_{r/2}^1(\hat{Q}_s)} \\ & \leq c \|\nabla \hat{u}\|_{W_r^1(\hat{Q}_s)} \leq c \|\hat{u}\|_{W_r^2(\hat{Q}_s)}, \end{aligned} \quad (5.42)$$

which follows from the continuity of the trace operator  $W_{r/2}^1(\hat{Q}_s) \rightarrow W_{r/2}^{1-2/r}(Y)$  and the continuity of the embedding  $W_{r/2}^{1-2/r}(Y) \hookrightarrow L_2(Y)$ , with  $r \geq 3$ .

The proof of the theorem will be performed in several steps:

**Step 1: Solve a linearized problem.**

For fixed  $\tilde{c}_s, \tilde{\phi} \in L_2(I \times Y)$ , replace  $f'(\phi) + \hat{q}(\phi, c_s, \hat{u})$  in (5.39) by

$$F(\tilde{c}_s, \tilde{\phi}) := f'(\tilde{\phi}) + \hat{q}(\tilde{\phi}, \tilde{c}_s, \hat{u}).$$

This leads to the following linearized problem:

Find  $c_s, \phi \in L_2(I; H_{per}^1(Y))$  with  $\partial_t c_s, \partial_t \phi \in L_2(I; H_{per}^1(Y)')$  such that the initial conditions (3.42) are satisfied and for every  $w_1, w_2 \in L_2(I; H_{per}^1(Y))$  the following equations

hold true:

$$\begin{aligned} \int_I \left( \tau \xi^2 \langle \partial_t \phi, w_1 \rangle + \int_Y \xi^2 \nabla \phi \cdot \nabla w_1 dy \right) dt \\ = - \int_{I \times Y} F(\tilde{c}_s, \tilde{\phi}) w_1 dy dt, \end{aligned} \quad (5.43)$$

$$\begin{aligned} \int_I \left( \langle \partial_t c_s, w_2 \rangle + \int_Y \left( D_s \nabla c_s \cdot \nabla w_2 + \frac{1}{\tau_s} c_s w_2 \right) dy \right) dt \\ = \int_I \left( \int_Y \frac{C^V}{\tau^V} w_2 dy - \varrho_s \langle \partial_t \phi, w_2 \rangle \right) dt. \end{aligned} \quad (5.44)$$

Note, that  $F$  is Lipschitz continuous with respect to  $c_s$  and  $\phi$ , see (5.38), and satisfies the growth condition

$$|F(c_s, \phi)| \leq c(\kappa) (1 + |\nabla \hat{u}|^2 + |c_s| + |\phi|),$$

see (5.37). Therefore,  $\tilde{c}_s, \tilde{\phi} \in L_2(I \times Y)$  implies  $F(\tilde{c}_s, \tilde{\phi}) \in L_2(I \times Y)$ . Equation (5.43) decouples from (5.44). It is, for given  $\tilde{c}_s$  and  $\tilde{\phi}$ , a weak formulation of a linear heat equation for  $\phi$ , independent of  $c_s$ . There exists a unique solution  $\phi \in L_2(I, H_{\text{per}}^1(Y))$  of (5.43) with  $\partial_t \phi \in L_2(I, H_{\text{per}}^1(Y)')$ , see [43], Theorem 11.3, p.382.

By the same reference, there is a unique solution  $c_s \in L_2(I, H_{\text{per}}^1(Y))$  with  $\partial_t c_s \in L_2(I, H_{\text{per}}^1(Y)')$  of (5.44), with the just found  $\partial_t \phi$  on the righthand side.

### Step 2: Estimates for the linearized problem.

Suppose  $\tilde{c}_{s,i}, \tilde{\phi}_i \in L_2(I \times Y)$ ,  $i = 1, 2$ , and let  $c_{s,i}, \phi_i$  be the corresponding solutions of (5.43), (5.44). Then the functions  $\check{c}_s := c_{s,1} - c_{s,2}$  and  $\check{\phi} := \phi_1 - \phi_2$  are solutions of

$$\begin{aligned} \int_I \tau \xi^2 \left( \langle \partial_t \check{\phi}, w_1 \rangle + \int_Y \xi^2 \nabla \check{\phi} \cdot \nabla w_1 dy \right) dt \\ = - \int_{I \times Y} (F(\tilde{c}_{s,1}, \tilde{\phi}_1) - F(\tilde{c}_{s,2}, \tilde{\phi}_2)) w_1 dy dt, \end{aligned} \quad (5.45)$$

$$\begin{aligned} \int_I \left( \langle \partial_t \check{c}_s, w_2 \rangle + \int_Y \left( D_s \nabla \check{c}_s \cdot \nabla w_2 + \frac{1}{\tau_s} \check{c}_s w_2 \right) dy \right) dt \\ = - \int_I \varrho_s \langle \partial_t \check{\phi}, w_2 \rangle dt, \end{aligned} \quad (5.46)$$

with  $\check{\phi}(0) = \check{c}_s(0) = 0$ . For  $z \in \{\check{c}_s, \check{\phi}\}$ , it is  $\partial_t \|z(t)\|_{L_2(Y)}^2 = 2 \langle \partial_t z, z \rangle(t)$  and thus

$$\int_0^{t_0} \langle \partial_t z, z \rangle dt = \frac{1}{2} (\|z(t_0)\|_{L_2(Y)}^2 - \|z(0)\|_{L_2(Y)}^2) = \frac{1}{2} \|z(t_0)\|_{L_2(Y)}^2, \quad (5.47)$$

for  $0 < t_0 \leq T$ . Set  $I_{t_0} = [0, t_0]$ . Taking  $w_1 = \chi_{I_{t_0}}(\phi_1 - \phi_2)$  in (5.45) and using the Lipschitz continuity of  $F$ , equation (5.47) and Young's inequality (2.1) yield

$$\begin{aligned} \|(\phi_1 - \phi_2)(t_0)\|_{L_2(Y)}^2 + \|\nabla(\phi_1 - \phi_2)\|_{L_2(I_{t_0} \times Y)}^2 \\ \leq c \left( \|\phi_1 - \phi_2\|_{L_2(I_{t_0} \times Y)}^2 + \|\tilde{c}_{s,1} - \tilde{c}_{s,2}\|_{L_2(I_{t_0} \times Y)}^2 + \|\tilde{\phi}_1 - \tilde{\phi}_2\|_{L_2(I_{t_0} \times Y)}^2 \right). \end{aligned} \quad (5.48)$$

This estimate also holds, if the gradient term on the left-hand side is neglected. Gronwall's inequality (2.4) then implies

$$\|\phi_1 - \phi_2\|_{L_\infty(I, L_2(Y))} \leq c \left( \|\tilde{c}_{s,1} - \tilde{c}_{s,2}\|_{L_2(I \times Y)} + \|\tilde{\phi}_1 - \tilde{\phi}_2\|_{L_2(I \times Y)} \right). \quad (5.49)$$

Due to the continuous embedding  $L_\infty(I, L_2(Y)) \hookrightarrow L_2(I \times Y)$ , it follows from (5.48) and (5.49)

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

and with (5.45)

$$\|\partial_t(\phi_1 - \phi_2)\|_{L_2(I, H^1(Y)')} \leq c \left( \|\tilde{c}_{s,1} - \tilde{c}_{s,2}\|_{L_2(I \times Y)} + \|\tilde{\phi}_1 - \tilde{\phi}_2\|_{L_2(I \times Y)} \right). \quad (5.50)$$

Setting  $w_2 = \chi_{I_{t_0}}(c_{s,1} - c_{s,2})$  in (5.46), it follows again with Young's inequality with  $\varepsilon > 0$  (2.2)

$$\begin{aligned} & \| (c_{s,1} - c_{s,2})(t_0) \|_{L_2(Y)}^2 + \| c_{s,1} - c_{s,2} \|_{L_2(I_{t_0}, H^1(Y))}^2 \\ & \leq \left| \int_{I_{t_0}} \langle \partial_t(\phi_1 - \phi_2), c_{s,1} - c_{s,2} \rangle dt \right| \\ & \leq c(\varepsilon) \|\partial_t(\phi_1 - \phi_2)\|_{L_2(I_{t_0}, H^1(Y)')}^2 + \varepsilon \|c_{s,1} - c_{s,2}\|_{L_2(I_{t_0}, H^1(Y))}^2, \end{aligned}$$

which implies together with (5.50) and for  $\varepsilon > 0$  small enough

$$\begin{aligned} & \|c_{s,1} - c_{s,2}\|_{L_\infty(I, L_2(Y))} + \|c_{s,1} - c_{s,2}\|_{L_2(I, H^1(Y))} \\ & \leq c \left( \|\tilde{c}_{s,1} - \tilde{c}_{s,2}\|_{L_2(I \times Y)} + \|\tilde{\phi}_1 - \tilde{\phi}_2\|_{L_2(I \times Y)} \right). \end{aligned} \quad (5.51)$$

An obvious consequence of the estimates (5.49) and (5.51) is

$$\begin{aligned} & \|\phi_1 - \phi_2\|_{L_\infty(I, L_2(Y))} + \|c_{s,1} - c_{s,2}\|_{L_\infty(I, L_2(Y))} \\ & \leq c \left( \|\tilde{c}_{s,1} - \tilde{c}_{s,2}\|_{L_2(I \times Y)} + \|\tilde{\phi}_1 - \tilde{\phi}_2\|_{L_2(I \times Y)} \right). \end{aligned} \quad (5.52)$$

### Step 3: Solve the original semi-linear problem using a fixed point argument.

Define the solution operator

$$\mathcal{F}: [L_\infty(I, L_2(Y))]^2 \rightarrow [L_\infty(I, L_2(Y))]^2: (\tilde{c}_s, \tilde{\phi}) \mapsto (c_s, \phi),$$

which maps given  $(\tilde{c}_s, \tilde{\phi})$  to the corresponding solutions of (5.43), (5.44). Note, that every function  $w \in L_\infty(I, L_2(Y))$  satisfies

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

This implies, together with estimate (5.52):

$$\begin{aligned} & \|\phi_1 - \phi_2\|_{L_\infty(I, L_2(Y))} + \|c_{s,1} - c_{s,2}\|_{L_\infty(I, L_2(Y))} \\ & \leq c T^{1/2} \left( \|\tilde{\phi}_1 - \tilde{\phi}_2\|_{L_\infty(I, L_2(Y))} + \|\tilde{c}_{s,1} - \tilde{c}_{s,2}\|_{L_\infty(I, L_2(Y))} \right). \end{aligned}$$

Choose  $0 < \tau_1 \leq T$  small enough, such that  $c\tau_1^{1/2} < 1$ . Then, restricted to the time interval  $I_{\tau_1} := [0, \tau_1]$ , the operator

$$\mathcal{F}: [L_\infty(I_{\tau_1}, L_2(Y))]^2 \rightarrow [L_\infty(I_{\tau_1}, L_2(Y))]^2$$

is a contraction. Banach's fixed point Theorem proves the existence of a unique solution  $(c_s, \phi)$  of (5.39), (5.40) on the possibly reduced time interval  $[0, \tau_1]$ . Since the choice of  $\tau_1$  is independent of the solution  $(c_s, \phi)$  and its initial data  $(c_{s,ini}, \phi_{ini})$ , finitely many repetitions of this arguments, with  $(c_s, \phi)(\tau_1)$  replacing the initial data, prove the existence of a solution on the whole time interval  $[0, T]$ .

#### Step 4: A priori estimate.

Proceed analogously to Step 2: Set  $w_1 = \chi_{I_{t_0}} \phi$  in (5.39). Use the growth condition (5.37) on  $f'$  and  $\hat{q}$

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

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

$$\begin{aligned} \|\phi(t_0)\|_{L_2(Y)}^2 + \|\nabla \phi\|_{L_2(I_{t_0} \times Y)}^2 &\leq c \left( 1 + \|\phi\|_{L_2(I_{t_0} \times Y)}^2 + \|c_s\|_{L_2(I_{t_0} \times Y)}^2 \right. \\ &\quad \left. + \|\nabla \hat{u}\|^2_{L_2(I_{t_0} \times Y)} + \|\phi_{ini}\|_{L_2(Y)}^2 \right). \end{aligned} \quad (5.53)$$

Gronwall's inequality implies

$$\|\phi\|_{L_\infty(I_{t_0}, L_2(Y))} \leq c (1 + \|c_s\|_{L_2(I_{t_0} \times Y)} + \|\nabla \hat{u}\|^2_{L_2(I_{t_0} \times Y)} + \|\phi_{ini}\|_{L_2(Y)}). \quad (5.54)$$

Estimate (5.53) leads first to

$$\|\phi\|_{L_2(I_{t_0}, H^1(Y))} \leq c (1 + \|\phi\|_{L_2(I_{t_0} \times Y)} + \|c_s\|_{L_2(I_{t_0} \times Y)} + \|\nabla \hat{u}\|^2_{L_2(I_{t_0} \times Y)} + \|\phi_{ini}\|_{L_2(Y)}), \quad (5.55)$$

next with the continuous embedding  $L_\infty(I_{t_0}, L_2(Y)) \hookrightarrow L_2(I_{t_0} \times Y)$  and (5.54) to

$$\|\phi\|_{L_2(I_{t_0}, H^1(Y))} \leq c (1 + \|c_s\|_{L_2(I_{t_0} \times Y)} + \|\nabla \hat{u}\|^2_{L_2(I_{t_0} \times Y)} + \|\phi_{ini}\|_{L_2(Y)}), \quad (5.56)$$

and finally with (5.39) to

$$\|\partial_t \phi\|_{L_2(I_{t_0}, H^1(Y))} \leq c (1 + \|c_s\|_{L_2(I_{t_0} \times Y)} + \|\nabla \hat{u}\|^2_{L_2(I_{t_0} \times Y)} + \|\phi_{ini}\|_{L_2(Y)}). \quad (5.57)$$

Set now  $w_2 = \chi_{I_{t_0}} c_s$  in (5.40) and use Young's inequality with  $\varepsilon > 0$  (2.2) to get

$$\begin{aligned} \|c_s(t_0)\|_{L_2(Y)}^2 + \|c_s\|_{L_2(I_{t_0}, H^1(Y))}^2 &\leq c \left( \|\partial_t \phi\|_{L_2(I_{t_0}, H^1(Y))} \|c_s\|_{L_2(I_{t_0}, H^1(Y))} + \|c_s\|_{L_2(I_{t_0} \times Y)}^2 \right. \\ &\quad \left. + \|C^\nu\|_{L_2(I_{t_0})}^2 + \|c_{s,ini}\|_{L_2(Y)}^2 \right) \\ &\leq c \left( c(\varepsilon) \|\partial_t \phi\|_{L_2(I_{t_0}, H^1(Y))}^2 + \varepsilon \|c_s\|_{L_2(I_{t_0}, H^1(Y))}^2 + \|c_s\|_{L_2(I_{t_0} \times Y)}^2 \right. \\ &\quad \left. + \|C^\nu\|_{L_2(I_{t_0})}^2 + \|c_{s,ini}\|_{L_2(Y)}^2 \right). \end{aligned} \quad (5.58)$$

Choosing  $\varepsilon$  small enough allows to cancel the  $\|c_s\|_{L_2(I_{t_0}, H^1(Y))}$ -term on the right-hand side of (5.58):

$$\begin{aligned} & \|c_s(t_0)\|_{L_2(Y)}^2 + \|c_s\|_{L_2(I_{t_0}, H^1(Y))}^2 \\ & \leq c \left( \|\partial_t \phi\|_{L_2(I_{t_0}, H^1(Y))}^2 + \|c_s\|_{L_2(I_{t_0} \times Y)}^2 + \|C^\nu\|_{L_2(I_{t_0})}^2 + \|c_{s,ini}\|_{L_2(Y)}^2 \right). \end{aligned}$$

Estimate (5.57) then yields

$$\begin{aligned} & \|c_s(t_0)\|_{L_2(Y)}^2 + \|c_s\|_{L_2(I_{t_0}, H^1(Y))}^2 \\ & \leq c \left( 1 + \|c_s\|_{L_2(I_{t_0} \times Y)}^2 + \|\nabla \hat{u}\|_{L_2(I_{t_0} \times Y)}^2 \right. \\ & \quad \left. + \|C^\nu\|_{L_2(I_{t_0})}^2 + \|c_{s,ini}\|_{L_2(Y)}^2 + \|\phi_{ini}\|_{L_2(Y)}^2 \right), \end{aligned} \quad (5.59)$$

and thus with Gronwall's inequality (2.4)

$$\|c_s\|_{L_\infty(I_{t_0}, L_2(Y))} \leq c \left( 1 + \|\nabla \hat{u}\|_{L_2(I_{t_0} \times Y)}^2 + \|C^\nu\|_{L_2(I_{t_0})} + \|c_{s,ini}\|_{L_2(Y)} + \|\phi_{ini}\|_{L_2(Y)} \right). \quad (5.60)$$

Combining (5.54), (5.56), (5.59) and (5.60) proves

$$\begin{aligned} & \|\phi\|_{L_\infty(I_{t_0}, L_2(Y))} + \|\phi\|_{L_2(I_{t_0}, H^1(Y))} + \|c_s\|_{L_\infty(I_{t_0}, L_2(Y))} + \|c_s\|_{L_2(I_{t_0}, H^1(Y))} \\ & \leq c \left( 1 + \|c_s\|_{L_2(I_{t_0} \times Y)} + \|\nabla \hat{u}\|_{L_2(I_{t_0} \times Y)} \right. \\ & \quad \left. + \|C^\nu\|_{L_2(I_{t_0})} + \|c_{s,ini}\|_{L_2(Y)} + \|\phi_{ini}\|_{L_2(Y)} \right). \end{aligned} \quad (5.61)$$

The embedding estimate

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

together with (5.42), (5.60) and (5.61) finally implies

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

for any  $0 < t_0 \leq T$ . Keep in mind, that  $c$  depends on  $\kappa$  from (5.37).  $\square$

**Theorem 5.19** (Regularity). *Suppose  $0 < \alpha < \frac{1}{2}$ ,  $r > \frac{6}{1-2\alpha}$  and  $\phi_{ini}, c_{s,ini} \in C_{\text{per}}^{2+2\alpha}(Y)$ , and consider given  $C^\nu \in C(I)$  and  $u$  with  $\hat{u} \in C(I, [W_{r,\text{per}}^2(\hat{Q}_s)]^3)$ . A solution  $(\phi, c_s)$  of (3.40), (3.41), (3.42) belongs to  $[C_{\text{per}}^{1,2+2\alpha}(I \times Y)]^2$  with*

$$\begin{aligned} & \|\phi(x)\|_{C^{1,2+2\alpha}(I \times Y)} + \|c_s(x)\|_{C^{1,2+2\alpha}(I \times Y)} \\ & \leq c(\kappa) \left( 1 + \|C^\nu(x)\|_{C(I)} + \|\hat{u}(x)\|_{C(I, W_r^2(\hat{Q}_s))}^2 \right. \\ & \quad \left. + \|\phi_{ini}(x)\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}(x)\|_{C^{2+2\alpha}(Y)} \right), \end{aligned} \quad (5.62)$$

with  $\kappa$  from (5.1).

*Proof.* As in the proof of Theorem 5.18, start again with analogous considerations on the coupling term:

Suppose  $\hat{u} \in [W_{r,\text{per}}^2(\hat{Q}_s)]^3$ , for fixed  $t$ , then:

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

For the norms there holds

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

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 [35] and Theorem 5.1.13 in [38], and perform a bootstrap procedure:

Let  $\Omega \subset \mathbb{R}^2$  be a bounded domain such that  $\bar{Y} \subset \Omega$  with  $C^{2+2\alpha}$ -smooth boundary  $\partial\Omega$ . Let  $\chi \in C_0^\infty(\Omega)$  be a cut-off function with  $\chi|_Y = 1$  and  $0 \leq \chi(y) \leq 1$  for all  $y \in \Omega$ . The functions  $\phi$  and  $c_s$  are  $Y$ -periodic in  $H^1(Y)$  which implies that they can be extended periodically to  $\Omega$  with  $\phi, c_s \in H^1(\Omega)$ . In the following, consider the functions  $\chi\phi$  and  $\chi c_s$ . If  $\phi$  and  $c_s$  solve (5.39) and (5.40) on  $I \times Y$ , then  $\chi\phi$  and  $\chi c_s$  are weak solutions of

$$\tau \xi^2 \partial_t(\chi\phi) - \xi^2 \Delta(\chi\phi) = -\chi(f'(\phi) + \hat{q}(c_s, \hat{u}, \phi)) - \xi^2(\phi \Delta \chi + 2\nabla \chi \nabla \phi), \quad (5.63)$$

$$\partial_t(\chi c_s) - D_s \Delta(\chi c_s) = \chi \left( \frac{C^V}{\tau^V} - \frac{c_s}{\tau_s} - \rho_s \partial_t \phi \right) - D_s(c_s \Delta \chi + 2\nabla \chi \nabla c_s) \quad (5.64)$$

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

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

where  $c_{s,ini}, \phi_{ini}$  are also extended periodically to  $\Omega$ . The weak formulation of (5.63) and (5.64) is analogous to that in (5.39) and (5.40). From  $c_s, \phi \in L_2(I, H^1(\Omega))$  it follows, that the righthand side of (5.63) is in  $L_2(I \times \Omega)$ , due to the growth condition (5.37) (This is also true if  $L_2$  is replaced by any  $L_\mu$ ,  $1 \leq \mu \leq \infty$ ). Omit again the dependency on  $\kappa$  in the following notation.

The application of Theorem 9.1 of Ch.IV in [35] yields

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

with

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

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

$$\|\phi\|_{W_2^{1,2}(I \times Y)} \leq c \left( 1 + \|\phi\|_{L_2(I, H^1(Y))} + \|c_s\|_{L_2(I \times Y)} + \|\hat{u}\|_{C(I, W_2^2(\hat{Q}_s))}^2 + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} \right). \quad (5.65)$$

The norms for  $\hat{u}$  and  $\phi_{ini}$  are not optimal at that point, but will be needed later anyway. Note, that (5.65) implies  $\partial_t \phi \in L_2(I \times Y)$ , so the righthand side of (5.64) is in  $L_2(I \times \Omega)$ . Theorem 9.1 of Ch.IV in [35] can now be applied to equation (5.64) and this yields

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

with

$$\|c_s\|_{W_2^{1,2}(I \times Y)} \leq c \left( \|c_s\|_{L_2(I, H^1(Y))} + \|\partial_t \phi\|_{L_2(I \times Y)} + \|C^\nu\|_{C(I)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)} \right). \quad (5.66)$$

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 Lemma 2.14. Furthermore, the embeddings

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

exist and are continuous, see Theorem 2.9, 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

$$\begin{aligned} &\|\phi\|_{W_4^{0,1}(I \times Y)} + \|c_s\|_{W_4^{0,1}(I \times Y)} \\ &\leq c \left( 1 + \|\phi\|_{L_2(I, H^1(Y))} + \|c_s\|_{L_2(I, H^1(Y))} + \|\hat{u}\|_{C(I, W_2^2(\hat{Q}_s))}^2 \right. \\ &\quad \left. + \|C^\nu\|_{C(I)} + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)} \right). \end{aligned} \quad (5.67)$$

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 (5.67) it follows

$$\begin{aligned} &\|\phi\|_{W_\mu^{0,1}(I \times Y)} + \|c_s\|_{W_\mu^{0,1}(I \times Y)} \\ &\leq c \left( 1 + \|\phi\|_{L_2(I, H^1(Y))} + \|c_s\|_{L_2(I, H^1(Y))} + \|\hat{u}\|_{C(I, W_2^2(\hat{Q}_s))}^2 \right. \\ &\quad \left. + \|C^\nu\|_{C(I)} + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)} \right). \end{aligned} \quad (5.68)$$

Another application of Theorem 9.1 of Ch.IV in [35] yields  $c_s, \phi \in W_\mu^{1,2}(I \times Y)$  for any  $1 \leq \mu < \infty$ , with

$$\begin{aligned} & \|\phi\|_{W_\mu^{1,2}(I \times Y)} + \|c_s\|_{W_\mu^{1,2}(I \times Y)} \\ & \leq c \left( 1 + \|\phi\|_{L_2(I, H^1(Y))} + \|c_s\|_{L_2(I, H^1(Y))} + \|\hat{u}\|_{C(I, W_\mu^2(\hat{Q}_s))}^2 \right. \\ & \quad \left. + \|C^\nu\|_{C(I)} + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)} \right). \end{aligned} \quad (5.69)$$

Use again the interpolatory inclusion

$$W_\mu^{1,2}(I \times Y) \hookrightarrow W_\mu^\lambda(I, W_\mu^{2(1-\lambda)}(Y)), \quad 0 < \lambda < 1, \quad (5.70)$$

with continuous embedding, see Lemma 2.14. 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  $2(1-\lambda) - \frac{2}{\mu} > 1 + 2\alpha$ , see Theorem 2.9. It follows that

$$W_\mu^\lambda(I, W_\mu^{2(1-\lambda)}(Y)) \hookrightarrow C(I, C^{1+2\alpha}(Y)), \quad (5.71)$$

for  $\mu > \frac{4}{1-2\alpha}$ ,  $0 < \alpha < \frac{1}{2}$ , with continuous embedding. So the right-hand side of (5.63) 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 [38] yields that  $\chi\phi \in C^{1,2+2\alpha}(I \times \Omega)$  with

$$\begin{aligned} \|\chi\phi\|_{C^{1,2+2\alpha}(I \times \Omega)} & \leq c \left( 1 + \|\chi\phi\|_{C^{0,1+2\alpha}(I \times \Omega)} + \|\chi c_s\|_{C^{0,2\alpha}(I \times \Omega)} \right. \\ & \quad \left. + \|\chi\hat{u}\|_{C(I, W_\mu^2(\hat{Q}_s))}^2 + \|\chi\phi_{ini}\|_{C^{2+2\alpha}(\Omega)} \right). \end{aligned} \quad (5.72)$$

Due to the just achieved regularity for  $\phi$ , the right-hand side of (5.64) 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 [38] with (5.72), it is  $\chi c_s \in C^{1,2+2\alpha}(I \times \Omega)$  with

$$\begin{aligned} \|\chi c_s\|_{C^{1,2+2\alpha}(I \times \Omega)} & \leq c \left( 1 + \|\chi\phi\|_{C^{0,1+2\alpha}(I \times \Omega)} + \|\chi c_s\|_{C^{0,1+2\alpha}(I \times \Omega)} \right. \\ & \quad \left. + \|\chi\hat{u}\|_{C(I, W_\mu^2(\hat{Q}_s))}^2 + \|C^\nu\|_{C(I)} \right. \\ & \quad \left. + \|\chi\phi_{ini}\|_{C^{2+2\alpha}(\Omega)} + \|\chi c_{s,ini}\|_{C^{2+2\alpha}(\Omega)} \right). \end{aligned} \quad (5.73)$$

The estimates (5.72) and (5.73), together with (5.41), (5.69), (5.70), (5.71) 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

$$\begin{aligned} & \|\phi\|_{C^{1,2+2\alpha}(I \times Y)} + \|c_s\|_{C^{1,2+2\alpha}(I \times Y)} \\ & \leq c \left( 1 + \|C^\nu\|_{C(I)} + \|\hat{u}\|_{C(I, W_\mu^2(\hat{Q}_s))}^2 + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)} \right). \end{aligned} \quad (5.74)$$

The constant  $c$  depends on  $\kappa$ , since the constant in the growth condition (5.37) does, which was used in the proof.  $\square$

**Remark 5.20.** Theorem 5.1.13 in [38], used in the previous proof, is an optimal regularity result for linear parabolic equations with Dirichlet boundary conditions, where the right-hand side is Hölder-continuous only in space. This is only an interior regularity result as counterexamples show, see [49]. For the boundary regularity, it is only true under the rather restrictive assumption, that the right-hand side vanishes on the boundary for every  $t \in I$ . Fortunately, it is satisfied here due to the cut-off by  $\chi$ .

**Lemma 5.21** (Continuity with respect to the coupling data). Suppose  $\hat{u}_1, \hat{u}_2 \in C(I, W_{r, \text{per}}^2(\hat{Q}_s))$  and  $C_1^\gamma, C_2^\gamma \in C(I)$ . Denote by  $\phi_1, \phi_2$  and  $c_{s,1}, c_{s,2}$  the corresponding solutions of (3.40)- (3.42). The continuity estimate

$$\begin{aligned} & \|(\phi_1 - \phi_2)(x)\|_{C^{1,2+2\alpha}(I \times Y)} + \|(c_{s,1} - c_{s,2})(x)\|_{C^{1,2+2\alpha}(I \times Y)} \\ & \leq c(\kappa) \left( \|(\hat{u}_1 + \hat{u}_2)(x)\|_{C(I, W_r^2(\hat{Q}_s))} \|(\hat{u}_1 - \hat{u}_2)(x)\|_{C(I, W_r^2(\hat{Q}_s))} \right. \\ & \quad \left. + \|(C_1^\gamma - C_2^\gamma)(x)\|_{C(I)} \right), \end{aligned} \quad (5.75)$$

holds true, with  $\kappa$  from sections 5.2.1 and 5.2.2.

*Proof.* The proof for the continuity estimate (5.75) is analogous to that for the a priori estimates (5.41) and (5.62) with the following adaptations: If  $\phi_1, \phi_2$  and  $c_{s,1}, c_{s,2}$  solve (3.40)- (3.42) with corresponding  $\hat{u}_1, \hat{u}_2$  and  $C_1^\gamma, C_2^\gamma$ , then

$$\tilde{\phi} := \phi_1 - \phi_2 \quad \text{and} \quad \tilde{c}_s := c_{s,1} - c_{s,2}$$

solve

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

with initial conditions

$$\tilde{c}_s(0, y) = 0, \quad \tilde{\phi}(0, y) = 0,$$

In order to imitate the proofs for estimates (5.41) and (5.62), the growth condition (5.37) for  $f'$  and  $q$  needs to be replaced by the Lipschitz condition (5.38). Furthermore, it is for  $r > \frac{6}{1-2\alpha}$

$$\begin{aligned} \|\nabla(\hat{u}_1 + \hat{u}_2) | \nabla(\hat{u}_1 - \hat{u}_2)\|_{C^{2\alpha}(Y)} &\leq c \|\nabla(\hat{u}_1 + \hat{u}_2) | \nabla(\hat{u}_1 - \hat{u}_2)\|_{W_{r/2}^{1-2/r}(Y)} \\ &\leq c \|\nabla(\hat{u}_1 + \hat{u}_2) | \nabla(\hat{u}_1 - \hat{u}_2)\|_{W_{r/2}^1(\hat{Q}_s)} \\ &\leq c \|\hat{u}_1 + \hat{u}_2\|_{W_r^2(\hat{Q}_s)} \|\hat{u}_1 - \hat{u}_2\|_{W_r^2(\hat{Q}_s)}. \end{aligned}$$

Proceeding as in the proofs for (5.41) and (5.62), using (5.38) instead of (5.37), finishes the proof.  $\square$

### 5.2.4 Microscopic Coupling

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 5.2.2 under the assumption that  $\phi(t, y) > 0$  for all  $t \in I$  and  $y \in \bar{Y}$ . Thus define

$$M := \left\{ \phi \in C(I, C_{\text{per}}^2(Y)) \mid \phi(t, y) > 0 \quad \forall t \in I, \forall y \in \bar{Y} \right\}.$$

Obviously,  $\phi \in M$  implies  $\phi(0, y) > 0$  for all  $y \in \bar{Y}$ . So the initial condition  $\phi_{ini}$  needs to satisfy  $\phi_{ini}(y) > 0$  for all  $y \in \bar{Y}$ . The results of the previous sections, namely Theorems 5.8, 5.14 and 5.19, allow the definition of the following solution operators:

$$\begin{aligned} \mathcal{S}_{\text{Stokes}} : & \begin{cases} M \times C(I, C_{\text{per}}^2(Y)) & \rightarrow C(I, [W_{r,\text{per}}^2(\hat{Q}_{IK})]^3 \times W_{r,\text{per}}^1(\hat{Q}_{IK})) \times M \\ (\phi, c_s) & \mapsto (\hat{v}, \hat{p}, \phi), \end{cases} \\ \mathcal{S}_{\text{elastic}} : & \begin{cases} C(I, [W_{r,\text{per}}^2(\hat{Q}_{IK})]^3 \times W_{r,\text{per}}^1(\hat{Q}_{IK})) \times M & \rightarrow C(I, [W_{r,\text{per}}^2(\hat{Q}_s)]^3) \\ (\hat{v}, \hat{p}, \phi) & \mapsto \hat{u}, \end{cases} \\ \mathcal{S}_{\text{phasefield}} : & \begin{cases} C(I, [W_{r,\text{per}}^2(\hat{Q}_s)]^3) & \rightarrow [C_{\text{per}}^{1,2+2\alpha}(I \times Y)]^2 \\ \hat{u} & \mapsto (\phi, c_s), \end{cases} \end{aligned}$$

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

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

has a unique fixed point. In order to apply Banach's fixed point theorem 2.18, it is necessary

- i) to find a suitable nonempty and closed subset  $B$  of  $M \times C(I, C_{\text{per}}^2(Y))$ , see Proposition 5.22, and
- ii) to show that  $\mathcal{S}$  maps  $B$  into itself, see Proposition 5.23, and
- iii) to show that  $\mathcal{S} : B \rightarrow B$  is a strict contraction, see Proposition 5.24.

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 Lemma 2.12, 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  $0 < \tau \leq T$  and set

$$M_{\tau,\alpha} := \left\{ \phi \in C^\alpha(I_\tau, C_{\text{per}}^2(Y)) \mid \phi(t, y) > 0 \quad \forall t \in I_\tau, \forall y \in \bar{Y} \right\}.$$

Define

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

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

**Proposition 5.22** (Well-definedness of  $\mathcal{S}$  on  $B_{R,\tau}$ ). *Suppose  $\phi_{ini}(y) > 0$  for all  $y \in \bar{Y}$ . For any  $R > \max\{\|\phi_{ini}\|_{C^2(Y)}, \|c_{s,ini}\|_{C^2(Y)}\}$  there exist a time  $\tau_1 > 0$ , depending on  $R$ , such that*

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

*Proof.* It is to show that  $(\phi, c_s) \in B_{R,\tau_1}$  implies  $\phi(t, y) > 0$  for all  $y \in \bar{Y}$  and  $t \leq \tau_1$ , 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,  $\phi$  is  $\alpha$ -Hölder continuous in time with Hölder constant  $\leq R$ . If  $\phi_{ini}(y) > 0$  for all  $y \in \bar{Y}$ , then there exists  $d := \min_{y \in \bar{Y}} \phi_{ini}(y) > 0$ , because  $\bar{Y}$  is compact. So,

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

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

Proposition 5.22 ensures that the operator

$$\mathcal{S}: B_{R,\tau_1} \rightarrow [C_{\text{per}}^{1,2+2\alpha}(I \times Y)]^2$$

is well defined. Furthermore, there is a configuration of  $R$  and  $\tau$ , such that  $\mathcal{S}$  maps  $B_{R,\tau}$  into itself:

**Proposition 5.23** (Self-mapping). *Suppose  $\phi_{ini}(y) > 0$  for all  $y \in \bar{Y}$ . There exist positive numbers  $R_0 > 0$  and  $\tau_2 > 0$  such that*

$$\mathcal{S}: B_{R_0,\tau_2} \rightarrow B_{R_0,\tau_2}.$$

$R_0$  and  $\tau_2$  depend on the macroscopic coupling data, the initial data and the boundary data for the Stokes system and the elasticity equation.

*Proof.* Suppose  $0 < \tau \leq \tau_1$ , with  $\tau_1$  from Proposition 5.22, 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  $\|\phi\|_{C^\alpha(I_\tau, C^2(Y))} + \|c_s\|_{C^\alpha(I_\tau, C^2(Y))} \leq R$ : The a priori estimates for the single parts of the problem, see Theorems 5.8, 5.14 and 5.19, imply that

$$\begin{aligned} & \|\phi\|_{C^{1,2+2\alpha}(I_\tau \times Y)} + \|c_s\|_{C^{1,2+2\alpha}(I_\tau \times Y)} \\ & \leq c(\kappa) \left( 1 + \|\tilde{c}_s\|_{C(I_\tau, C^2(Y))}^2 + \|C^\nu\|_{C(I_\tau)}^2 + \|\nabla_x V\|_{C(I_\tau)}^2 \right. \\ & \quad \left. + \|P\|_{C(I_\tau)}^2 + \|b\|_{C(I_\tau, W_r^{2-1/r}(Y \times \{0\}))}^2 + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)} \right), \end{aligned} \quad (5.76)$$

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

$$\|\tilde{\phi}(t, y) - \phi_{ini}(y)\|_{C^2(Y)} \leq R t^\alpha \leq \frac{d}{2},$$

and thus

$$\sup_{t \in I_\tau} \|\tilde{\phi}(t)\|_{C^2(Y)} \leq \|\phi_{ini}\|_{C^2(Y)} + \frac{d}{2} =: \kappa.$$

So, the constant  $c$  in (5.76) can be chosen independently of  $\tilde{\phi}$  and  $R$ , and (5.76) can be written as

$$\begin{aligned} & \|\phi\|_{C^{1,2+2\alpha}(I_\tau \times Y)} + \|c_s\|_{C^{1,2+2\alpha}(I_\tau \times Y)} \\ & \leq c_1(C^\nu, V, P, b, \phi_{ini}, c_{s,ini}) + c_2 \|\tilde{c}_s\|_{C(I_\tau, C^2(Y))}^2, \end{aligned} \quad (5.77)$$

where

$$\begin{aligned} c_1(C^\nu, V, P, b, \phi_{ini}, c_{s,ini}) = & c \left( 1 + \|C^\nu\|_{C(I)}^2 + \|\nabla_x V\|_{C(I)}^2 + \|P\|_{C(I)}^2 + \|\phi_{ini}\|_{C^{2+2\alpha}(Y)} \right. \\ & \left. + \|c_{s,ini}\|_{C^{2+2\alpha}(Y)} + \|b\|_{C(I, W_r^{2-1/r}(Y \times \{0\}))}^2 \right). \end{aligned}$$

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, (5.77) becomes

$$\|\phi\|_{C^{1,2+2\alpha}(I_\tau \times Y)} + \|c_s\|_{C^{1,2+2\alpha}(I_\tau \times Y)} \leq \tilde{c}_1(C^\nu, V, P, b, \phi_{ini}, c_{s,ini}) + \tilde{c}_2 R^2 \tau^{2\alpha}, \quad (5.78)$$

with

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

The continuous embedding

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

see Lemma 2.12, implies together with (5.78) that

$$\begin{aligned} \|\phi\|_{C^\alpha(I_\tau, C^2(Y))} + \|c_s\|_{C^\alpha(I_\tau, C^2(Y))} &\leq c_3 \left( \|\phi\|_{C^{1,2+2\alpha}(I_\tau \times Y)} + \|c_s\|_{C^{1,2+2\alpha}(I_\tau \times Y)} \right) \\ &\leq c_3 \tilde{c}_1(C^\nu, V, P, b, \phi_{ini}, c_{s,ini}) + c_3 \tilde{c}_2 R^2 \tau^{2\alpha}. \end{aligned} \quad (5.79)$$

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 (5.79) 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  $\tau$  such that

$$\mathcal{S}: B_{R,\tau} \rightarrow B_{R,\tau}$$

is a strict contraction:

**Proposition 5.24** (Contraction). *Consider  $R_0$  from Proposition 5.23. There exists a number  $\tau_3 > 0$  such that the operator*

$$\mathcal{S}: B_{R_0,\tau_3} \rightarrow B_{R_0,\tau_3}$$

*is a strict contraction.*

*Proof.* Suppose  $0 < \tau \leq \tau_2$ , with  $\tau_2$  from Proposition 5.23, 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 5.9, 5.15 and 5.21 (with  $C_1^\nu = C_2^\nu$ ) imply that

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

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 5.23,  $\kappa$  can be chosen independently of  $\tilde{\phi}_i \in B_{R_0,\tau}$ , if  $\tau \leq \tau_1$ , with  $\tau_1$  from Proposition 5.22. This is satisfied here. Furthermore, the a priori estimates of Theorems 5.8 and 5.14 yield together with  $(\tilde{\phi}_i, \tilde{c}_{s,i}) \in B_{R_0,\tau}$

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

This leads to

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

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

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

The continuous embedding

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

see Lemma 2.12, implies

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

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

So at last, everything is prepared to prove the solvability of the coupled microscopic problem as the most important result in section 5.2. It is formulated in the following theorem:

**Theorem 5.25** (Existence and uniqueness of a solution of the coupled microscopic problem). *Suppose  $C^\nu(x, \cdot)$ ,  $\nabla_x V(x, \cdot)$ ,  $P(x, \cdot) \in C(I_{\tau_3})$  for  $x \in S_0$ , with  $\tau_3$  from Proposition 5.24. Assume furthermore that*

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

with  $\phi_{ini}(x, y) > 0$  for all  $y \in \bar{Y}$ . Then, there exists a unique solution  $(\phi, c_s, v, p, u)(x)$  of (3.33) – (3.42) with

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

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

$$\begin{aligned} & \|\phi(x)\|_{C^{1,2+2\alpha}(I_{\tau_3} \times Y)} + \|c_s(x)\|_{C^{1,2+2\alpha}(I_{\tau_3} \times Y)} + \|\hat{v}(x)\|_{C(I_{\tau_3}, W_{r,\text{per}}^2(\hat{Q}_{IK}))} \\ & \quad + \|\hat{p}(x)\|_{C(I_{\tau_3}, W_{r,\text{per}}^1(\hat{Q}_{IK}))} + \|\hat{u}(x)\|_{C(I_{\tau_3}, W_{r,\text{per}}^2(\hat{Q}_s))} \\ & \leq c \left( 1 + \|C^{\nu}(x)\|_{C(I_{\tau_3})}^2 + \|\nabla_x V(x)\|_{C(I_{\tau_3})}^2 + \|P(x)\|_{C(I_{\tau_3})}^2 \right. \\ & \quad \left. + \|b(x)\|_{C(I_{\tau_3}, W_r^{2-1/r}(Y \times \{0\}))}^2 + \|\phi_{\text{ini}}(x)\|_{C^{2+2\alpha}(Y)} + \|c_{s,\text{ini}}(x)\|_{C^{2+2\alpha}(Y)} \right). \end{aligned} \quad (5.80)$$

*Proof.* The assumptions for Banach's fixed point theorem, see 2.18, on the operator

$$\mathcal{S}: B_{R_0, \tau_3} \rightarrow B_{R_0, \tau_3}$$

are fulfilled and so, there exists a unique fixed point in  $B_{R_0, \tau_3}$ . Any fixed point  $(\phi, c_s)$  of  $\mathcal{S}$ , together with

$$(\hat{v}, \hat{p}) = \mathcal{S}_{\text{Stokes}}(\phi, c_s), \quad \hat{u} = \mathcal{S}_{\text{elastic}}(\hat{v}, \hat{p}, \phi)$$

solves (3.33) – (3.42). Due to Theorems 5.8, 5.14 and 5.19, it is

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

As seen in Proposition 5.23,  $(\phi, c_s)$  satisfy

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

and by the definition of  $R_0$  in the proof of Proposition 5.23 and the estimates of Lemmata 5.8 and 5.14 it follows (5.80).

It remains to show that the just found solution is unique not only in  $B_{R_0, \tau_3}$ , but also in  $M \times C(I_{\tau_3}, C_{\text{per}}^2(Y))$ . Suppose therefore that  $(\phi_i, c_{s,i}) \in M \times C(I_{\tau_3}, C_{\text{per}}^2(Y))$ ,  $i = 1, 2$ , are fixed points of  $\mathcal{S}$ . Note, that  $(\phi_i, c_{s,i})$  also belong to  $C_{\text{per}}^{1,2+2\alpha}(I_{\tau_3} \times Y)$ , due to Theorems 5.8, 5.14 and 5.19, and thus to  $C^\alpha(I_{\tau_3}, C_{\text{per}}^2(Y))$ . Since  $(\phi_i, c_{s,i})$  satisfy the same initial condition, it is  $\|(\phi_1 - \phi_2)(0)\|_{C^2(Y)} = \|(c_{s,1} - c_{s,2})(0)\|_{C^2(Y)} = 0$ . As seen in Proposition 5.24, the estimate

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

is satisfied for any  $\tau \in I_{\tau_3}$ , where  $\kappa \geq \max\{\|\phi_1\|_{C(I_{\tau_3}, C^2(Y))}, \|\phi_2\|_{C(I_{\tau_3}, C^2(Y))}\}$ . 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

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

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  $\|(\phi_1 - \phi_2)(t)\|_{C^2(\mathcal{Y})} = \|(c_{s,1} - c_{s,2})(t)\|_{C^2(\mathcal{Y})} = 0$  for all  $t \in [t_0, t_0 + \tau(t_0)] \cap I_{\tau_3}$ . This shows that the set

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

is an open subset of  $I_{\tau_3}$ , and it is not empty because  $0 \in I'$ . But since  $t \mapsto \|(\phi, c_s)(t)\|_{C^2(\mathcal{Y})}$  is continuous,  $I'$  is also closed in  $I_{\tau_3}$  and therefore  $I' = I_{\tau_3}$ . This proves uniqueness of the solution of (3.33) – (3.42).  $\square$

With the statement of Theorem 5.25, the main goal concerning the analysis for the microscopic problem is reached. Until here, a macroscopic point  $x \in S_0$  was fixed. This sections 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 5.26** (Regularity with respect to  $x \in S_0$ ). *Suppose that  $C^\mathcal{V}$ ,  $\nabla_x V$ ,  $P$ ,  $b$ ,  $\phi_{ini}$  and  $c_{s,ini}$  depend continuously on  $x \in S_0$ . Then, the solution of (3.33) – (3.42) depends continuously on  $x \in S_0$  and*

$$\begin{aligned} & \|\phi\|_{C(S_0, C^{1,2+2\alpha}(I_{\tau_3} \times \mathcal{Y}))} + \|c_s\|_{C(S_0, C^{1,2+2\alpha}(I_{\tau_3} \times \mathcal{Y}))} + \|\hat{V}\|_{C(I_{\tau_3} \times S_0, W_{r,per}^2(\hat{Q}_{IK}))} \\ & \quad + \|\hat{\rho}\|_{C(I_{\tau_3} \times S_0, W_{r,per}^1(\hat{Q}_{IK}))} + \|\hat{u}\|_{C(I_{\tau_3} \times S_0, W_{r,per}^2(\hat{Q}_s))} \\ & \leq c \left( 1 + \|C^\mathcal{V}\|_{C(I_{\tau_3} \times S_0)}^2 + \|b\|_{C(I_{\tau_3} \times S_0, W_r^{2-1/r}(\mathcal{Y} \times \{0\}))}^2 + \|\nabla_x V\|_{C(I_{\tau_3} \times S_0)}^2 \right. \\ & \quad \left. + \|P\|_{C(I_{\tau_3} \times S_0)}^2 + \|\phi_{ini}\|_{C(S_0, C^{2+2\alpha}(\mathcal{Y}))} + \|c_{s,ini}\|_{C(S_0, C^{2+2\alpha}(\mathcal{Y}))} \right). \end{aligned} \quad (5.81)$$

*Proof.* Suppose for  $i = 1, 2$  points  $x_i \in S_0$  and set  $C_i^\mathcal{V} = C^\mathcal{V}(x_i)$ ,  $\phi_i = \phi(x_i)$  and  $c_{s,i} = c_s(x_i)$ . Analogously to the proof of Proposition 5.24 it holds for  $\tau \in I_{\tau_3}$

$$\begin{aligned} & \|\phi_1 - \phi_2\|_{C^\alpha(I_\tau, C^2(\mathcal{Y}))} + \|c_{s,1} - c_{s,2}\|_{C^\alpha(I_\tau, C^2(\mathcal{Y}))} \\ & \leq c \left( \tau^\alpha (\|\phi_1 - \phi_2\|_{C^\alpha(I_\tau, C^2(\mathcal{Y}))} + \|c_{s,1} - c_{s,2}\|_{C^\alpha(I_\tau, C^2(\mathcal{Y}))}) + \|C_1^\mathcal{V} - C_2^\mathcal{V}\|_{C(I_\tau)} \right), \end{aligned} \quad (5.82)$$

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

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

Repeating these arguments, starting with arbitrary  $t_0 \in I_{\tau_3}$  as initial time, leads to an analogous estimate as (5.82) on the time interval  $[t_0, t_0 + \tau] \cap I_{\tau_3}$ , with a constant  $\tilde{c}$  depending on  $\|\phi_i(t_0)\|_{C^{2+2\alpha}(\mathcal{Y})}$  and  $\|c_{s,i}(t_0)\|_{C^{2+2\alpha}(\mathcal{Y})}$  instead of  $\|\phi_i(0)\|_{C^{2+2\alpha}(\mathcal{Y})}$  and  $\|c_{s,i}(0)\|_{C^{2+2\alpha}(\mathcal{Y})}$ . Thanks to the a priori estimate (5.80), the mentioned constant  $\tilde{c}$  can in fact be chosen independently of  $t_0$ , such that

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

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

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

with a constant  $c > 0$  depending only on the initial, boundary and macroscopic coupling data. The right hand side tends to zero for  $|x_1 - x_2| \rightarrow 0$ , since  $C^\mathcal{V}$  is continuous with respect to  $x$ . It follows that  $\phi$ ,  $c_s$  and, due to Lemmata 5.9, 5.15, 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 (5.80) to prove (5.81).  $\square$

**Lemma 5.27** (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 (3.33) – (3.42). These solutions depend locally Lipschitz continuous on  $C_1^\mathcal{V}$  and  $C_2^\mathcal{V}$ , i.e. if  $\|C_i^\mathcal{V}\|_{C(I_{\tau_3} \times S_0)} \leq R$ , for some  $R > 0$ , then*

$$\begin{aligned} & \|\phi_1 - \phi_2\|_{C(S_0, C^{1,2+2\alpha}(I_{\tau_3} \times Y))} + \|c_{s,1} - c_{s,2}\|_{C(S_0, C^{1,2+2\alpha}(I_{\tau_3} \times Y))} \\ & + \|\hat{v}_1 - \hat{v}_2\|_{C(I_{\tau_3} \times S_0, W_{r,\text{per}}^2(\hat{Q}_{IK}))} + \|\hat{p}_1 - \hat{p}_2\|_{C(I_{\tau_3} \times S_0, W_{r,\text{per}}^1(\hat{Q}_{IK}))} \\ & + \|\hat{u}_1 - \hat{u}_2\|_{C(I_{\tau_3} \times S_0, W_{r,\text{per}}^2(\hat{Q}_s))} \\ & \leq c \|C_1^\mathcal{V} - C_2^\mathcal{V}\|_{C(I_{\tau_3} \times S_0)}, \end{aligned} \quad (5.83)$$

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

*Proof.* Consider first fixed  $x \in S_0$ . Analogously to the proof of Lemma 5.26 it holds

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

with a constant  $c > 0$  depending only on the initial, boundary and macroscopic coupling data. The continuity estimates of Lemmata 5.9 and 5.15 then imply

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

Taking the maximum with respect to  $x \in S_0$  proves (5.83).  $\square$

**Remark 5.28.** *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, which is an obvious consequence of the Lemmata 5.26 and 5.27, is stated explicitly:

**Lemma 5.29** (On the microscopic mean value  $\bar{c}_s$ ). *It holds*

$$\begin{aligned} \|\bar{c}_s\|_{C^1(I_{\tau_3}, C(S_0))} \leq & c \left( 1 + \|C^\nu\|_{C(I_{\tau_3} \times S_0)}^2 + \|\nabla_x V\|_{C(I_{\tau_3} \times S_0)}^2 + \|P\|_{C(I_{\tau_3} \times S_0)}^2 \right. \\ & + \|b\|_{C(I_{\tau_3} \times S_0, W_r^{2-1/r}(Y \times \{0\}))}^2 + \|\phi_{ini}\|_{C(S_0, C^{2+2\alpha}(Y))} \\ & \left. + \|c_{s,ini}\|_{C(S_0, C^{2+2\alpha}(Y))}^2 \right), \end{aligned}$$

and

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

with the same constant  $c > 0$  as in Lemma 5.27.

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

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

The statements follow from

$$|\bar{f}(x, t)| = \left| \int_Y f(x, t, y) dy \right| \leq \|f(x, t)\|_{C(Y)} \int_Y 1 dy, \quad f \in \{c_s, \partial_t c_s\},$$

and  $|Y| = 1$  and estimates (5.81) and (5.83) respectively. □

### 5.3 Solvability of the Macroscopic Equations

The macroscopic part of the two scale model consists of the Navier-Stokes equations (3.25) with boundary and initial conditions (3.28), (3.30), (3.32), and the convection-diffusion equation (3.26) with boundary and initial conditions (3.27), (3.29), (3.31). These equations are posed on  $I \times Q$ , where  $Q$  has the form of a container, as introduced in chapter 3, 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  $C^\beta(I, C(\bar{Q}))$  throughout this section, with some  $\beta > 0$ . It remains to investigate the convection-diffusion problem with  $\bar{c}_s$  as coupling datum. The following **weak formulation** of the problem has already been investigated in [17]:

**Problem 5.30.** Find  $C^\nu \in L_2(I, H^1(Q))$  with  $\partial_t C^\nu \in L_2(I, H^1(Q)')$  such that the initial condition  $C^\nu(0, x) = C_{ini}^\nu(x)$  is satisfied for almost all  $x \in Q$  and that for every  $w \in L_2(I; H^1(Q))$

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

where  $\langle \cdot, \cdot \rangle$  denotes the dual pairing in  $H^1(Q)$ .

This problem has a unique solution:

**Theorem 5.31.** Suppose  $V \in L_\infty(I, L_2(Q)) \cap L_2(I, H^1(Q))$  is a solution of the Navier-Stokes equations (3.25), (3.28), (3.30), (3.32), and  $\bar{c}_s \in L_2(I \times S_0)$ ,  $C_{ini}^\nu \in L_2(Q)$ . Assume further that  $D^\nu > 0$ ,  $\tau^\nu > 0$ . Then, problem 5.30 has a unique solution.

*Proof.* The statement follows from [35], chapter III, Theorem 5.1, see also [17].  $\square$

Unfortunately, the regularity properties for  $C^\nu$  which are ensured by Theorem 5.31 are not good enough for the coupling to the microscopic problem:

- **Space regularity:** Lemma 5.26 supposes  $C^\nu(\cdot, t) \in C(S_0)$ , see also Remark 5.28. If  $C^\nu(\cdot, t) \in H^1(Q)$  as in Theorem 5.31, then  $C^\nu(\cdot, t) \in H^{1/2}(S_0)$  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 5.2 in spaces of continuous functions in time, because uniform in time bounds for  $\|\phi(t)\|_{C^2(\gamma)}$  are needed there. This is proven under the condition that also the coupling quantity  $C^\nu$  is continuous in time, i.e.  $C^\nu(x, \cdot) \in C(I)$ . In fact, if  $C^\nu \in L_2(I, H^1(Q))$  with  $\partial_t C^\nu \in L_2(I, H^1(Q)')$  as proven in Theorem 5.31, then  $C^\nu \in C(I, L_2(Q))$ , see [43], Lemma 11.4, p.383, but  $C^\nu \in C(I \times S_0)$  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 (3.27), (3.29). A solution in  $W_r^2(Q)$  or even  $C^2(Q)$  or  $C^{2+\alpha}(Q)$  can not be expected. The coming discussion pursues the following strategy:

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

- Consider the corresponding stationary problem

$$-D^\nu \Delta C^\nu + V \cdot \nabla C^\nu = 0, \quad \text{in } Q, \quad (5.84)$$

$$D^\nu \frac{\partial C^\nu}{\partial n} = \begin{cases} \frac{\bar{c}_s}{\tau_s} - \frac{C^\nu}{\tau^\nu}, & \text{on } S_0, \\ 0, & \text{on } \partial Q \setminus S_0. \end{cases} \quad (5.85)$$

Prove the existence of a unique weak solution  $C^\nu \in W_r^1(Q)$ , see Theorems 5.36 and 5.37. The weak formulation (see problem 5.34 on page 95) of (5.84), (5.85) can be written as

$$-AC^\nu = \ell_{c_s},$$

with  $\ell_{c_s}$  depending on  $c_s$  and an operator

$$A(t): W_r^1(Q) \rightarrow (W_{r'}^1(Q))', \quad \text{with } \frac{1}{r} + \frac{1}{r'} = 1, \quad (5.86)$$

defined in (5.89).  $A = A(t)$  depends on  $t$ , because  $V$  depends on  $t$ .

- Study the eigenvalue problem

$$-A(t)C^\nu + \lambda C^\nu = \ell,$$

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 5.38 and 5.39.

- Use semigroup theory to prove the existence and uniqueness of a solution  $C^\nu \in C(I, W_r^1(Q))$  of

$$\partial_t C^\nu = A(t)C^\nu + \ell_{c_s}, \quad \text{in } I = [0, T], \quad C^\nu(0) = C_{ini}^\nu,$$

(see Theorem 5.40), which is a reformulation of the convection-diffusion problem (3.26), (3.27), (3.29), (3.31).

**Remark 5.32.** *In the case, where the stationary problem (5.84), (5.85) has smooth solutions in  $W_r^2(Q)$  or  $C^{2+\alpha}(Q)$ , all of the three just mentioned items are covered by well-known literature as for example [38]. The case of non-smooth solutions (of the stationary problem) is less considered in the literature. Here, in the study of the regularity of the solution of the stationary problem, a result from the recently published textbook [39] is used. The following results are new, to the best of the author's knowledge.*

### The stationary problem

Suppose  $1 < r, r' < \infty$  with  $\frac{1}{r} + \frac{1}{r'} = 1$ ,  $w \in W_{r'}^1(Q)$ . Multiply equation (5.84) by  $w$  and integrate by parts to get

$$\int_Q (D^\nu \nabla C^\nu \cdot \nabla w + V \cdot \nabla C^\nu w) dx + \int_{S_0} \frac{1}{\tau^\nu} C^\nu w ds = \int_{S_0} \frac{1}{\tau_s} \bar{c}_s w ds.$$

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

$$\begin{aligned} \int_Q V \cdot \nabla C^\nu w dx &= \int_{\partial Q} C^\nu w \underbrace{V \cdot n}_{=0} ds - \int_Q C^\nu \operatorname{div}(wV) dx \\ &= - \int_Q \left( C^\nu w \underbrace{\operatorname{div} V}_{=0} + C^\nu V \cdot \nabla w \right) dx \\ &= - \int_Q C^\nu V \cdot \nabla w dx \end{aligned}$$

Define

$$a(C^\nu, w) := \int_Q (D^\nu \nabla C^\nu \cdot \nabla w - C^\nu V \cdot \nabla w) dx + \int_{S_0} \frac{1}{\tau^\nu} C^\nu w ds, \quad (5.87)$$

$$\langle \ell_{c_s}, w \rangle := \int_{S_0} \frac{1}{\tau_s} \bar{c}_s w ds, \quad (5.88)$$

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

**Lemma 5.33.** *Suppose  $\bar{c}_s \in C(S_0)$  and  $1 \leq r' \leq \infty$ . Then,  $\ell_{c_s} \in (W_{r'}^1(Q))'$  with*

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

*Proof.* It is

$$\int_{S_0} |\bar{c}_s w| ds \leq \|\bar{c}_s\|_{C(S_0)} \int_{S_0} |w| ds.$$

The continuous embedding  $W_{r'}^{1-\frac{1}{r'}}(S_0) \hookrightarrow L_1(S_0)$ , see Theorem 2.9, and the continuity of the trace operator, see Theorem 2.2, yield

$$\int_{S_0} |w| ds \leq c \|w\|_{W_{r'}^{1-\frac{1}{r'}}(S_0)} \leq c \|w\|_{W_{r'}^1(Q)}.$$

Finally

$$\langle \ell_{c_s}, w \rangle \leq c \|\bar{c}_s\|_{C(S_0)} \|w\|_{W_{r'}^1(Q)},$$

which proves the result.  $\square$

The operator  $A$  in (5.86) is defined by

$$A: W_r^1(Q) \rightarrow (W_{r'}^1(Q))' : AC^\nu := -a(C^\nu, \cdot), \quad (5.89)$$

with  $a$  form (5.87). Note that  $A = A(t)$  depends on time, since  $V$  depends on time, which will be important when discussing the evolution problem.

A **weak formulation** for (5.84), (5.85) is:

**Problem 5.34.** Find  $C^\nu \in W_r^1(Q)$  such that

$$a(C^\nu, w) = \langle \ell_{c_s}, w \rangle,$$

for all  $w \in W_{r'}^1(Q)$ .

**Lemma 5.35.** The bilinear form  $a: W_r^1(Q) \times W_{r'}^1(Q) \rightarrow \mathbb{R}$  is continuous.

*Proof.* The continuity of the trace operator, see Theorem 2.2, the continuous embeddings  $W_\rho^{1-\frac{1}{p}}(S_0) \hookrightarrow L_\rho(S_0)$ ,  $\rho \in \{r, r'\}$ , see Theorem 2.9, and Hölder's inequality (2.3) imply

$$\begin{aligned} \int_{S_0} C^\nu w \, ds &\leq \|C^\nu\|_{L_r(S_0)} \|w\|_{L_{r'}(S_0)} \\ &\leq \|C^\nu\|_{W_r^{1-\frac{1}{r}}(S_0)} \|w\|_{W_{r'}^{1-\frac{1}{r'}}(S_0)} \\ &\leq c \|C^\nu\|_{W_r^1(Q)} \|w\|_{W_{r'}^1(Q)}, \end{aligned}$$

and again with Hölder's inequality

$$\begin{aligned} a(C^\nu, w) &\leq D^\nu \|\nabla C^\nu\|_{L_r(Q)} \|\nabla w\|_{L_{r'}(Q)} \\ &\quad + \|V\|_{L_\infty(Q)} \|C^\nu\|_{L_r(Q)} \|\nabla w\|_{L_{r'}(Q)} + \frac{1}{\tau^\nu} \|C^\nu\|_{L_r(S_0)} \|w\|_{L_{r'}(S_0)} \\ &\leq c \|C^\nu\|_{W_r^1(Q)} \|w\|_{W_{r'}^1(Q)}. \end{aligned}$$

□

There is a unique weak solution for the stationary convection-diffusion problem in the Hilbert-space-case  $r = r' = 2$ :

**Theorem 5.36** (Solvability of the stationary problem in  $H^1(Q)$ ). Suppose  $\bar{c}_s \in C(S_0)$ ,  $D^\nu, \tau^\nu > 0$  and  $r = r' = 2$ . Then, there is a unique solution of Problem 5.34 in  $H^1(Q)$ .

*Proof.* In order to apply the Lax-Milgram theorem 2.17, it remains to prove (in addition to the Lemmata 5.33 and 5.35), that the bilinear form  $a$  is  $H^1(Q)$ -elliptic, i.e. there is a constant  $c > 0$  such that

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

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

$$\int_Q V \cdot \nabla C^\nu C^\nu \, dx = \int_Q V \cdot \frac{1}{2} \nabla |C^\nu|^2 \, dx = \int_{\partial Q} \frac{1}{2} |C^\nu|^2 \underbrace{V \cdot n}_{=0} \, ds - \int_Q \frac{1}{2} C^\nu \underbrace{\operatorname{div} V}_{=0} \, dx = 0.$$

So,  $a(C^\nu, C^\nu)$  reduces to

$$a(C^\nu, C^\nu) = \int_Q D^\nu |\nabla C^\nu|^2 \, dx + \int_{S_0} \frac{1}{\tau^\nu} |C^\nu|^2 \, ds. \quad (5.90)$$

In fact,

$$\|C^\nu\|_a := \left( \int_Q D^\nu |\nabla C^\nu|^2 \, dx + \int_{S_0} \frac{1}{\tau^\nu} |C^\nu|^2 \, ds \right)^{\frac{1}{2}}$$

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 [58], pp.247-248. This proves  $H^1(Q)$ -ellipticity of  $a$ .  $\square$

For the discussion of the regularity of the solution, the mixed boundary value problem (5.84), (5.85) can be rewritten as a Neumann problem, as described in the proof of the following theorem:

**Theorem 5.37** (Regularity/Solvability of the stationary problem in  $W_r^1(Q)$ ). *Suppose  $\bar{c}_s \in C(S_0)$  and  $C^\nu \in H^1(Q)$  is the unique solution of Problem 5.34 for  $r = r' = 2$ . Then  $C^\nu \in W_r^1(Q)$  for any  $r \geq 2$ . Furthermore,  $C^\nu$  is the unique solution of Problem 5.34 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 5.34 is equivalent to the weak formulation of the following Neumann problem:

$$\begin{aligned} -\Delta C^\nu &= F(C^\nu), & \text{in } Q, \\ \frac{\partial C^\nu}{\partial n} &= 0, & \text{on } \partial Q, \end{aligned}$$

with

$$\langle F(C^\nu), w \rangle := \int_Q C^\nu V \cdot \nabla w \, dx - \int_{S_0} \frac{1}{\tau^\nu} C^\nu w \, ds + \langle \ell_{c_s}, w \rangle. \quad (5.91)$$

If  $F(C^\nu) \in (W_{r'}^1(Q))'$ , then the weak solution of the above Neumann problem, and therefore the solution of problem 5.34, belongs to  $W_r^1(Q)$ , thanks to [39], Theorem 8.3.10, p.377.

In order to prove  $F(C^\nu) \in (W_{r'}^1(Q))'$ , suppose  $w \in W_{r'}^1(Q)$  and study every term in (5.91) separately:

- $C^\nu \in H^1(Q)$  implies  $C^\nu \in L_6(Q)$ , see Theorem 2.9. Due to Hölder's inequality, the volume integral is finite, if  $\nabla w \in L_{\frac{6}{5}}(Q)$ , i.e. for  $r' \geq \frac{6}{5}$ .
- $C^\nu \in H^1(Q)$  implies  $C^\nu \in H^{\frac{1}{2}}(S_0)$ , see Theorem 2.2, and  $H^{\frac{1}{2}}(S_0) \hookrightarrow L_4(S_0)$ , see Theorem 2.9. So the boundary integral in (5.91) is finite, if  $w \in L_{\frac{4}{3}}(S_0)$ , due to Hölder's inequality.  $w \in W_r^1(Q)$  implies  $w \in W_{r'}^{1-\frac{1}{r'}}(S_0)$ , see Theorem 2.2, and  $W_{r'}^{1-\frac{1}{r'}}(S_0) \hookrightarrow L_{\frac{4}{3}}(S_0)$  for  $r' \geq \frac{6}{5}$ , see Theorem 2.9.
- The last term is finite for any  $r' \geq 1$ , due to Lemma 5.33.

It follows that  $F(C^\nu) \in (W_r^1(Q))'$  for  $r' \geq \frac{6}{5}$ , and thus  $C^\nu \in W_r^1(Q)$  for  $r \leq 6$ . This result can be improved by repeating the same arguments, starting from  $C^\nu \in W_6^1(Q)$  instead of  $C^\nu \in H^1(Q)$ . Suppose again  $w \in W_{r'}^1(Q)$ . Then:

- $C^\nu \in W_6^1(Q)$  implies  $C^\nu \in L_\infty(Q)$ , see Theorem 2.9. So the volume integral is finite, if  $\nabla w \in L_1(Q)$ , which is true for any  $r' \geq 1$ .
- $C^\nu \in W_6^1(Q)$  implies  $C^\nu \in W_6^{\frac{5}{6}}(S_0)$ , see Theorem 2.2, and  $W_6^{\frac{5}{6}}(S_0) \hookrightarrow L_\infty(S_0)$ , see Theorem 2.9. So the boundary integral in (5.91) is finite, if  $w \in L_1(S_0)$  which is given for any  $r' \geq 1$ , see Theorem 2.2.

Consequently  $C^\nu$  belongs to  $W_r^1(Q)$  and satisfies

$$a(C^\nu, w) = \langle \ell_{c_s}, w \rangle,$$

for all  $w \in H^1(Q)$  by assumption. Since  $H^1(Q)$  is dense in  $W_r^1(Q)$ , which follows from Theorem 2.3,  $C^\nu$  solves Problem 5.34 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: A solution for  $r \geq 2$  also is a solution for  $r = 2$ . The solution for  $r = 2$  is unique, and so is that for  $r \geq 2$ .  $\square$

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

The study of the evolution equation

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

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  $A: D(A) \subset X \rightarrow X$  with domain  $D(A)$ . As special case,  $X = L_r(\Omega)$  and  $D(A) \subseteq W_r^2(\Omega)$  is treated for example in [38] and [41], 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 (5.89), for fixed  $t_0 \in I$ , is sectorial for  $X = (W_r^1(Q))'$  and  $D(A) = W_r^1(Q)$ , and generates an analytic semigroup on  $(W_r^1(Q))'$ .

So, consider in the following the operator  $A = A(t_0)$  at fixed  $t_0 \in I$ .

**Lemma 5.38.** *The resolvent set  $\rho(A)$  contains the complex half plane  $\{\lambda \in \mathbb{C} : \operatorname{Re} \lambda \geq 0\}$ .*

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

$$-AC^\nu + \lambda C^\nu = \ell. \quad (5.92)$$

Equation (5.92) is an equation in  $(W_r^1(Q))'$ , so  $C^\nu \in W_r^1(Q)$  is understood as an element of  $(W_r^1(Q))'$  by setting

$$\langle C^\nu, w \rangle := \int_Q C^\nu w \, dx, \quad \forall w \in W_r^1(Q).$$

Then (5.92) can be written as

$$a_\lambda(C^\nu, w) := a(C^\nu, w) + \lambda \int_Q C^\nu w \, dx = \langle \ell, w \rangle, \quad \forall w \in W_r^1(Q). \quad (5.93)$$

In the Hilbert space case  $r = r' = 2$ , the bilinear form  $a_\lambda$  is obviously continuous and also  $H^1(Q)$ -elliptic if  $\lambda \geq 0$ . Therefore, there exists for each  $\ell \in (H^1(Q))'$  a unique  $C^\nu \in H^1(Q)$  solving (5.93), due to the Lax-Milgram theorem. A repetition of the arguments in the proof of Theorem 5.37 yields that  $C^\nu$  belongs to  $W_r^1(Q)$  and is the unique solution of (5.93) for any  $r \geq 2$ .

For complex  $\lambda$  the bilinear forms  $a$  and  $a_\lambda$  have to be understood as sesquilinear forms:

$$\begin{aligned} a(C^\nu, w) &= \int_Q \left( \overline{D^\nu \nabla C^\nu} \cdot \nabla w + \overline{C^\nu V} \cdot \nabla w \right) dx + \int_{S_0} \overline{\frac{1}{\tau^\nu} C^\nu w} \, ds, \\ a_\lambda(C^\nu, w) &= a(C^\nu, w) + \lambda \int_Q \overline{C^\nu w} \, dx. \end{aligned}$$

For  $r = r' = 2$ , the ellipticity condition on  $a_\lambda$  in the Lax-Milgram theorem reads

$$\operatorname{Re} (a_\lambda(C^\nu, C^\nu)) \geq c \|C^\nu\|_{H^1(Q)}^2,$$

see [4], Theorem 4.2, p.164. This is satisfied if  $\operatorname{Re} \lambda \geq 0$ . It follows, that there exists for each  $\ell \in (H^1(Q))'$  a unique  $C^\nu \in W_r^1(Q)$  solving (5.93), if  $\operatorname{Re} \lambda \geq 0$ .

Concluding, it is proven that for  $\operatorname{Re} \lambda \geq 0$  the operator

$$-A + \lambda \mathbf{I} : W_r^1(Q) \rightarrow (W_r^1(Q))',$$

is linear and continuous, due to the continuity of  $a_\lambda$ , and bijective, due to the existence and uniqueness of the solution of (5.93). By the bounded inverse theorem, see [43], Theorem 8.34, pp.241, the inverse

$$(-A + \lambda \mathbf{I})^{-1} : (W_r^1(Q))' \rightarrow W_r^1(Q),$$

is linear and bounded, i.e. the solution  $C^\nu$  of (5.93) satisfies the a priori estimate

$$\|C^\nu\|_{W_r^1(Q)} \leq c \|\ell\|_{(W_r^1(Q))'}. \quad (5.94)$$

Furthermore, the resolvent operator  $R(\lambda, A) = (-A + \lambda \mathbf{I})^{-1}$  belongs to  $L((W_r^1(Q))')$ , which implies that  $\lambda \in \rho(A)$ .  $\square$

**Lemma 5.39.** For  $\lambda \in \mathbb{C}$  with  $\operatorname{Re} \lambda \geq 0$ , the resolvent  $R(\lambda, A)$  satisfies the estimate

$$\|\lambda R(\lambda, A)\|_{L((W_r^1(Q))')} \leq c,$$

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

*Proof.* Consider  $\ell \in (W_r^1(Q))'$  and suppose that  $C^\nu = R(\lambda, A) \ell$  is the corresponding solution of (5.93). Then

$$\begin{aligned} \|\lambda R(\lambda, A) \ell\|_{(W_r^1(Q))'} &= \|\lambda C^\nu\|_{(W_r^1(Q))'} \\ &= \sup_{\substack{w \in W_r^1(Q), \\ \|w\|_{W_r^1(Q)}=1}} \lambda \langle C^\nu, w \rangle \\ &= \sup_{\substack{w \in W_r^1(Q), \\ \|w\|_{W_r^1(Q)}=1}} (a_\lambda(C^\nu, w) - a(C^\nu, w)) \\ &\stackrel{(5.93)}{\leq} \|\ell\|_{(W_r^1(Q))'} + \sup_{\substack{w \in W_r^1(Q), \\ \|w\|_{W_r^1(Q)}=1}} a(C^\nu, w) \\ &\stackrel{\text{Lemma 5.35}}{\leq} \|\ell\|_{(W_r^1(Q))'} + c \|C^\nu\|_{W_r^1(Q)} \\ &\stackrel{(5.94)}{\leq} \tilde{c} \|\ell\|_{(W_r^1(Q))'}. \end{aligned}$$

Due to Proposition 2.19,  $A$  is sectorial. □

### The evolution problem

Turn back to the nonstationary convection-diffusion problem

$$\partial_t C^\nu = A(t)C^\nu + \ell_{cs}, \quad \text{in } I = [0, T], \quad C^\nu(0) = C_{ini}^\nu. \quad (5.95)$$

The spatial differential operator  $A$  is treated in a weak formulation, while the time derivative has to be understood in the classical sense.

Problem (5.95) 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 [38], since the time dependency of  $A$  only occurs in its coefficients for lower order terms. The exact procedure is explained in the proof of the following theorem, the most important result of this section:

**Theorem 5.40** (Existence and uniqueness of a solution of the macroscopic problem). *Suppose  $r \geq 2$ ,  $C_{ini}^\nu \in W_r^1(Q)$ ,  $\bar{c}_s \in C^\beta(I, C(S_0))$  and  $V \in C^\beta(I, C(\bar{Q}))$  for some  $\beta > 0$ . Then, there exists a unique solution  $C^\nu \in C^1(I, (W_r^1(Q))') \cap C(I, W_r^1(Q))$  of (5.95) satisfying the a priori estimate*

$$\|C^\nu\|_{C(I, W_r^1(Q))} + \|C^\nu\|_{C^1(I, (W_r^1(Q))')} \leq c (\|\bar{c}_s\|_{C^\beta(I, C(S_0))} + \|C_{ini}^\nu\|_{W_r^1(Q)}). \quad (5.96)$$

*Proof.* Assume w.l.o.g.  $\beta \leq \frac{1}{r}$ .

The differential equation in (5.95) can be rewritten as

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

To shorten the notation during the proof set

$$W = C^1(I, (W_r^1(Q))') \cap C(I, W_r^1(Q)), \quad \|\cdot\|_W := \|\cdot\|_{C(I, W_r^1(Q))} + \|\cdot\|_{C^1(I, (W_r^1(Q))')}$$

Define

$$W_0 = \{\varphi \in W \mid \varphi(0) = C_{ini}^\nu\}.$$

Suppose  $\tilde{C}^\nu \in W_0$  and consider

$$\partial_t C^\nu = A(0)C^\nu + (A(t) - A(0))\tilde{C}^\nu + \ell_{c_s}, \quad C^\nu(0) = C_{ini}^\nu, \quad (5.97)$$

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

- for any  $\tilde{C}^\nu \in W_0$  there exists a unique solution  $C^\nu$  of (5.97) and
- the mapping  $\mathcal{F}: W_0 \rightarrow W_0: \tilde{C}^\nu \mapsto C^\nu$  has a unique fixed point.

Start by discussing the regularity of the right hand side terms in (5.97):

$$\begin{aligned} \langle (A(t) - A(0))\tilde{C}^\nu, w \rangle &= \int_Q \tilde{C}^\nu (V(0) - V(t)) \cdot \nabla w \, dx \\ &\leq \|V(0) - V(t)\|_{C(Q)} \|\tilde{C}^\nu\|_{L_r(Q)} \|w\|_{W_r^1(Q)}. \end{aligned} \quad (5.98)$$

Due to Lemma 2.16 it is  $\tilde{C}^\nu \in C^{\frac{1}{r}}(I, L_r(Q))$  and so it follows from (5.98) and from  $\beta \leq \frac{1}{r}$  that  $(A(t) - A(0))\tilde{C}^\nu \in C^\beta(I, (W_r^1(Q))')$  with

$$\|(A(t) - A(0))\tilde{C}^\nu\|_{C^\beta(I, (W_r^1(Q))')} \leq \|V\|_{C^\beta(I, C(\bar{Q}))} \|\tilde{C}^\nu\|_{C^\beta(I, L_r(Q))}.$$

Lemma 5.33 and  $\bar{c}_s \in C^\beta(I, C(S_0))$  implies  $\ell_{c_s} \in C^\beta(I, (W_r^1(Q))')$  with

$$\|\ell_{c_s}\|_{C^\beta(I, (W_r^1(Q))')} \leq c \|\bar{c}_s\|_{C^\beta(I, C(S_0))}.$$

Note furthermore that  $W_r^1(Q)$  is dense in  $(W_r^1(Q))'$ , see Lemma 2.6. Thus all the assumptions of [38], Theorem. 4.3.1.(ii) are satisfied and there exists a unique solution  $C^\nu \in W_0$  of (5.97) for any  $\tilde{C}^\nu \in W_0$  with

$$\begin{aligned} \|C^\nu\|_W &\leq c \left( \|(A(t) - A(0))\tilde{C}^\nu + \ell_{c_s}\|_{C^\beta(I, (W_r^1(Q))')} + \|C_{ini}^\nu\|_{W_r^1(Q)} \right) \\ &\leq c \left( \|\tilde{C}^\nu\|_{C^\beta(I, L_r(Q))} + \|\bar{c}_s\|_{C^\beta(I, C(S_0))} + \|C_{ini}^\nu\|_{W_r^1(Q)} \right). \end{aligned}$$

Problem (5.97) is linear and thus, if  $C_1^\nu, C_2^\nu \in W_0$  are the respective solutions for  $\tilde{C}_1^\nu, \tilde{C}_2^\nu \in W_0$ , then

$$\partial_t(C_1^\nu - C_2^\nu) = A(0)(C_1^\nu - C_2^\nu) + (A(t) - A(0))(\tilde{C}_1^\nu - \tilde{C}_2^\nu), \quad (C_1^\nu - C_2^\nu)(0) = 0,$$

with

$$\|C_1^\nu - C_2^\nu\|_W \leq c \|\tilde{C}_1^\nu - \tilde{C}_2^\nu\|_{C^\beta(I, L_r(Q))}. \quad (5.99)$$

This and the embedding of  $W$  into  $C^{\frac{1}{r}}(I, L_r(Q))$ , see Lemma 2.16, show that the mapping

$$\mathcal{F}: W_0 \rightarrow W_0: \tilde{C}^\nu \mapsto C^\nu$$

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  $\tilde{C}_1^\nu, \tilde{C}_2^\nu \in W_0$  satisfy

$$\begin{aligned} \|\tilde{C}_1^\nu - \tilde{C}_2^\nu\|_{C^\beta(I_\tau, L_r(Q))} &\leq c\tau^{\beta_1 - \beta} \|\tilde{C}_1^\nu - \tilde{C}_2^\nu\|_{C^{\beta_1}(I_\tau, L_r(Q))} \\ &\leq c\tau^{\beta_1 - \beta} \|\tilde{C}_1^\nu - \tilde{C}_2^\nu\|_W, \end{aligned} \quad (5.100)$$

due to  $\tilde{C}_1^\nu(0) = \tilde{C}_2^\nu(0)$ . Estimates (5.99) and (5.100) with  $\tau$  small enough prove

$$\|\mathcal{F}(\tilde{C}_1^\nu) - \mathcal{F}(\tilde{C}_2^\nu)\|_W \leq c \|\tilde{C}_1^\nu - \tilde{C}_2^\nu\|_W,$$

with a constant  $c < 1$ . Banach's fixed point Theorem implies that there exists a unique solution of (5.95) in  $W_0$  on a possibly reduced time interval  $I_\tau$ .

It is possible to repeat the procedure, starting from  $\tau$  as new initial time. In fact, this proves existence and uniqueness of a solution of (5.95) 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  $C_{ini}^\nu$  has no influence on the constants but the sectorial operator  $A(0)$  in (5.97) has, when applying [38], Theorem 4.3.1.(ii), see also the remarks in the beginning of chapter 4 in [38], 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  $\tau$  independently of the initial time.

As conclusion, finitely many repetitions of the described method prove existence and uniqueness of a solution of (5.95) in  $W_0$  on the whole time interval  $I$ .

The **a priori estimate** (5.96) is proven as follows: Consider again the time interval  $I_\tau$ , for which  $\mathcal{F}$  is a contraction. Denote by  $C^\nu$  the unique solution of (5.95), which is a fixed point of  $\mathcal{F}$ , and by  $\tilde{C}_{ini}^\nu$  the function in  $W_0$  which is constant in time, i.e.  $\tilde{C}_{ini}^\nu(t) = C_{ini}^\nu, \forall t$ . Then

$$\begin{aligned} \|C^\nu - \tilde{C}_{ini}^\nu\|_W &= \|\mathcal{F}(C^\nu) - \mathcal{F}(\tilde{C}_{ini}^\nu) + \mathcal{F}(\tilde{C}_{ini}^\nu) - \tilde{C}_{ini}^\nu\|_W \\ &\leq \|\mathcal{F}(C^\nu) - \mathcal{F}(\tilde{C}_{ini}^\nu)\|_W + \|\mathcal{F}(\tilde{C}_{ini}^\nu) - \tilde{C}_{ini}^\nu\|_W \\ &\leq c \|C^\nu - \tilde{C}_{ini}^\nu\|_W + \|\mathcal{F}(\tilde{C}_{ini}^\nu) - \tilde{C}_{ini}^\nu\|_W, \end{aligned}$$

with  $c < 1$ , and therefore

$$\|C^\nu - \tilde{C}_{ini}^\nu\|_W \leq c \|\mathcal{F}(\tilde{C}_{ini}^\nu) - \tilde{C}_{ini}^\nu\|_W, \quad (5.101)$$

with some  $c > 0$ .  $\tilde{C}_{ini}^\nu$  is constant in time and therefore

$$\begin{aligned} \|(A(t) - A(0)) \tilde{C}_{ini}^\nu\|_{C^\beta(I_\tau, (W_r^1(Q))')} &\leq \|V\|_{C^\beta(I_\tau, C(\bar{Q}))} \|\tilde{C}_{ini}^\nu\|_{C^\beta(I_\tau, L_r(Q))} \\ &= \|V\|_{C^\beta(I_\tau, C(\bar{Q}))} \|\tilde{C}_{ini}^\nu\|_{C(I_\tau, L_r(Q))} \\ &\leq \|V\|_{C^\beta(I_\tau, C(\bar{Q}))} \|C_{ini}^\nu\|_{W_r^1(Q)}. \end{aligned}$$

$\mathcal{F}(\tilde{C}_{ini}^\nu)$  is by definition the solution of (5.97) with  $\tilde{C}_{ini}^\nu$  on the right-hand side, and thus satisfies due to [38], Theorem. 4.3.1.(ii)

$$\begin{aligned} \|\mathcal{F}(\tilde{C}_{ini}^\nu)\|_W &\leq c \left( \|(A(t) - A(0)) \tilde{C}_{ini}^\nu + \ell_{c_s}\|_{C^\beta(I_\tau, (W_r^1(Q))')} + \|C_{ini}^\nu\|_{W_r^1(Q)} \right) \\ &\leq c \left( \|C_{ini}^\nu\|_{W_r^1(Q)} + \|\bar{c}_s\|_{C^\beta(I_\tau, C(S_0))} \right). \end{aligned} \quad (5.102)$$

Combining (5.101), (5.102) with

$$\|\tilde{C}_{ini}^\nu\|_W \leq \|C_{ini}^\nu\|_{W_r^1(Q)},$$

leads to

$$\begin{aligned} \|C^\nu\|_W &\leq \|C^\nu - \tilde{C}_{ini}^\nu\|_W + \|\tilde{C}_{ini}^\nu\|_W \\ &\leq c \|\mathcal{F}(\tilde{C}_{ini}^\nu) - \tilde{C}_{ini}^\nu\|_W + \|C_{ini}^\nu\|_{W_r^1(Q)} \\ &\leq c \left( \|\mathcal{F}(\tilde{C}_{ini}^\nu)\|_W + \|\tilde{C}_{ini}^\nu\|_W \right) + \|C_{ini}^\nu\|_{W_r^1(Q)} \\ &\leq c \left( \|\bar{c}_s\|_{C^\beta(I_\tau, C(S_0))} + \|C_{ini}^\nu\|_{W_r^1(Q)} \right) \end{aligned} \quad (5.103)$$

Estimate (5.103) is valid on the reduced time interval  $I_\tau$ . In particular it implies

$$\|C^\nu(\tau)\|_{W_r^1(Q)} \leq c \left( \|\bar{c}_s\|_{C^\beta(I_\tau, C(S_0))} + \|C_{ini}^\nu\|_{W_r^1(Q)} \right).$$

Therefore, an iteration of these arguments, replacing  $C_{ini}^\nu$  by  $C^\nu(\tau)$  proves (5.96).  $\square$

**Lemma 5.41** (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  $C_1^\nu, C_2^\nu$  the corresponding solutions of (5.95). Then*

$$\|C_1^\nu - C_2^\nu\|_{C(I, W_r^1(Q))} + \|C_1^\nu - C_2^\nu\|_{C^1(I, (W_r^1(Q))')} \leq c \|\bar{c}_{s,1} - \bar{c}_{s,2}\|_{C^\beta(I, C(S_0))}. \quad (5.104)$$

*Proof.* The coupling to the microscopic problem is linear, i.e.

$$\ell_{c_{s,1}} - \ell_{c_{s,2}} = \ell_{c_{s,1} - c_{s,2}}.$$

Furthermore, problem (5.95) is linear and thus  $C_1^\nu - C_2^\nu$  solves

$$\partial_t(C_1^\nu - C_2^\nu) = A(t)(C_1^\nu - C_2^\nu) + \ell_{c_{s,1} - c_{s,2}}, \quad (C_1^\nu - C_2^\nu)(0) = 0,$$

in  $I = [0, T]$ . Theorem 5.40 implies (5.104).  $\square$

## 5.4 Micro-Macro-Coupling: Proof of the Main Result

After investigating the microscopic part of the model in section 5.2 and the macroscopic part in section 5.3, their coupling can now be discussed. The most important results of the previous sections are shortly recapitulated here:

For given  $C^\nu \in C(I \times S_0)$  there exists locally in time a unique solution of the microscopic part of the problem (3.33) – (3.42), see Theorem 5.25. This microscopic solution satisfies in particular  $\bar{c}_s \in C^1(I_{\tau_3}, C(S_0))$ , with  $\tau_3$  from Theorem 5.25, and

$$\begin{aligned} \|\bar{c}_s\|_{C^1(I_{\tau_3}, C(S_0))} &\leq c \left( 1 + \|C^\nu\|_{C(I_{\tau_3} \times S_0)}^2 + \|\nabla_x V\|_{C(I_{\tau_3} \times S_0)}^2 + \|P\|_{C(I_{\tau_3} \times S_0)}^2 \right. \\ &\quad + \|b\|_{C(I_{\tau_3} \times S_0, W_r^{2-1/r}(\bar{\Gamma}))}^2 + \|\phi_{ini}\|_{C(S_0, C^{2+2\alpha}(Y))} \\ &\quad \left. + \|c_{s,ini}\|_{C(S_0, C^{2+2\alpha}(Y))}^2 \right). \end{aligned} \quad (5.105)$$

Furthermore,  $\bar{c}_s$  depends locally Lipschitz continuous on  $C^\nu$ , i.e. if  $C_1^\nu, C_2^\nu \leq R$ , then

$$\|\bar{c}_{s,1} - \bar{c}_{s,2}\|_{C^1(I_{\tau_3}, C(S_0))} \leq c \|C_1^\nu - C_2^\nu\|_{C(I_{\tau_3} \times S_0)}, \quad (5.106)$$

with a constant  $c$  depending on  $R$ , see Lemma 5.27.

Conversely, for given  $\bar{c}_s \in C^\beta(I, C(S_0))$ , with some  $\beta > 0$ , there exists a unique solution  $C^\nu \in C^1(I, (W_{r'}^1(Q))') \cap C(I, W_r^1(Q))$  of the macroscopic problem (3.26), (3.27), (3.29), (3.31), with  $r \geq 2$ , depending continuously on  $\bar{c}_s$  and satisfying

$$\|C^\nu\|_{C(I, W_r^1(Q))} + \|C^\nu\|_{C^1(I, (W_{r'}^1(Q))')} \leq c (\|\bar{c}_s\|_{C^\beta(I, C(S_0))} + \|C_{ini}^\nu\|_{W_r^1(Q)}), \quad (5.107)$$

and

$$\|C_1^\nu - C_2^\nu\|_{C(I, W_r^1(Q))} + \|C_1^\nu - C_2^\nu\|_{C^1(I, (W_{r'}^1(Q))')} \leq c \|\bar{c}_{s,1} - \bar{c}_{s,2}\|_{C^\beta(I, C(S_0))}, \quad (5.108)$$

see Theorem 5.40 and Lemma 5.41.

On this basis relies the proof of the main result of this thesis, Theorem 5.1, which is stated here again:

**Theorem** (Existence and uniqueness of solutions of the fully coupled problem). *Suppose  $V \in C^\beta(I, C(\bar{Q})) \cap C(I, C^1(\bar{Q}))$ , for some  $\beta > 0$ , and  $P \in C(I \times \bar{Q})$  are solutions of the Navier-Stokes equations (3.25), (3.28), (3.30) and (3.32). Assume furthermore that  $\phi_{ini}, c_{s,ini} \in C(S_0, C_{\text{per}}^{2+2\alpha}(Y))$ , with  $\phi_{ini}(y) > 0$  for all  $y \in \bar{Y}$ ,  $b \in C(I \times S_0, W_{r_1, \text{per}}^{2-1/r_1}(\bar{\Gamma}))$  and  $C_{ini}^\nu \in W_{r_2}^1(Q)$ , 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 (3.26), (3.27), (3.29), (3.31) and (3.33) – (3.42) in the following function spaces:*

$$\begin{aligned} \hat{v} &\in C(I_{\tau_0} \times S_0, W_{r_1, \text{per}, \text{loc}}^2(\hat{Q}_I)), & \phi &\in C(S_0, C_{\text{per}}^{1, 2+2\alpha}(I_{\tau_0} \times Y)), \\ \hat{p} &\in C(I_{\tau_0} \times S_0, W_{r_1, \text{per}, \text{loc}}^1(\hat{Q}_I)), & c_s &\in C(S_0, C_{\text{per}}^{1, 2+2\alpha}(I_{\tau_0} \times Y)), \\ \hat{u} &\in C(I_{\tau_0} \times S_0, W_{r_1, \text{per}}^2(\hat{Q}_s)), & C^\nu &\in C^1\left(I_{\tau_0}, (W_{r_2}^1(Q))'\right) \cap C\left(I_{\tau_0}, W_{r_2}^1(Q)\right). \end{aligned}$$

*Proof.* Consider the time interval  $I_\tau = [0, \tau]$  and suppose that  $\tau$  is small enough to guarantee the existence of a solution of the microscopic problem on  $I_\tau$ , i.e.  $\tau \leq \tau_3$ , compare Theorem 5.25. Note that for  $r_2 > 3$ , the space  $W_{r_2}^1(Q)$  is continuously embedded into  $C(\bar{Q})$ , see Theorem 2.9, and thus

$$C^\nu \in C(I_\tau, W_{r_2}^1(Q)) \implies C^\nu \in C(I_\tau \times \bar{Q}) \implies C^\nu|_{S_0} \in C(I_\tau \times S_0).$$

Define the solution operators

$$\begin{aligned} \mathcal{L}_{\text{micro}}: C(I_\tau \times \bar{Q}) &\rightarrow C^1(I_\tau, C(S_0)): C^\nu \mapsto \bar{c}_s, \\ \mathcal{L}_{\text{macro}}: C^\beta(I_\tau, C(S_0)) &\rightarrow C(I_\tau \times \bar{Q}) \quad : \bar{c}_s \mapsto C^\nu, \end{aligned}$$

and their composition

$$\mathcal{L} := \mathcal{L}_{\text{macro}} \circ \mathcal{L}_{\text{micro}}: C(I_\tau \times \bar{Q}) \rightarrow C(I_\tau \times \bar{Q}): \tilde{C}^\nu \mapsto C^\nu.$$

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

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

and thus

$$\begin{aligned} \|\bar{c}_s\|_{C^\beta(I_\tau, C(S_0))} &= \|\bar{c}_s\|_{C(I_\tau \times S_0)} + \sup_{t_1 \neq t_2 \in I_\tau} \frac{\|\bar{c}_s(t_1) - \bar{c}_s(t_2)\|_{C(S_0)}}{|t_1 - t_2|^\beta} \\ &\leq c \left( \tau^{1-\beta} \|\bar{c}_s\|_{C^1(I_\tau, C(S_0))} + \|\bar{c}_{s,ini}\|_{C(S_0)} \right). \end{aligned} \quad (5.109)$$

For  $\tilde{C}^\nu \in C(I_\tau \times \bar{Q})$ , set  $C^\nu := \mathcal{L}(\tilde{C}^\nu)$ . Estimates (5.105) and (5.107), combined with (5.109) and the continuous embedding  $C(I_\tau, W_{r_2}^1(Q)) \hookrightarrow C(I_\tau \times \bar{Q})$  imply

$$\begin{aligned} \|C^\nu\|_{C(I_\tau \times \bar{Q})} &\leq c \|C^\nu\|_{C(I_\tau, W_{r_2}^1(Q))} \\ &\leq c \left( \|\bar{c}_s\|_{C^\beta(I_\tau, C(S_0))} + \|C_{ini}^\nu\|_{W_{r_2}^1(Q)} \right) \\ &\leq c \left( \tau^{1-\beta} \|\bar{c}_s\|_{C^1(I_\tau, C(S_0))} + \|\bar{c}_{s,ini}\|_{C(S_0)} + \|C_{ini}^\nu\|_{W_{r_2}^1(Q)} \right) \\ &\leq c_1(V, P, b, C_{ini}^\nu, \phi_{ini}, c_{s,ini}) + c_2 \tau^{1-\beta} \|\tilde{C}^\nu\|_{C(I_\tau \times \bar{Q})}^2, \end{aligned} \quad (5.110)$$

with a constant  $c_2 > 0$  and

$$\begin{aligned} c_1(V, P, b, C_{ini}^\nu, \phi_{ini}, c_{s,ini}) &= c \left( 1 + \|\nabla_x V\|_{C(I_{\tau_3} \times S_0)}^2 + \|P\|_{C(I_{\tau_3} \times S_0)}^2 \right. \\ &\quad \left. + \|b\|_{C(I_{\tau_3} \times S_0, W_{r_1}^{2-1/r_1}(\bar{r}))}^2 + \|\phi_{ini}\|_{C(S_0, C^{2+2\alpha}(\Upsilon))} \right. \\ &\quad \left. + \|c_{s,ini}\|_{C(S_0, C^{2+2\alpha}(\Upsilon))}^2 + \|C_{ini}^\nu\|_{W_{r_2}^1(Q)} \right). \end{aligned} \quad (5.111)$$

Choose  $M_0 := 2c_1$  and define

$$B_\tau = \left\{ \tilde{C}^\nu \in C(I_\tau \times \bar{Q}) \mid \|\tilde{C}^\nu\|_{C(I_\tau \times \bar{Q})} \leq M_0, \tilde{C}^\nu(x, 0) = C_{ini}^\nu(x), \forall x \in \bar{Q} \right\}.$$

Then, estimate (5.110) and  $M_0 = 2c_1$  imply that  $\mathcal{L}$  maps  $B_\tau$  into itself as long as

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

In order to apply Banach's fixed point Theorem on

$$\mathcal{L}: B_\tau \rightarrow B_\tau,$$

combine estimates (5.106) and (5.108) to get

$$\|C_1^\mathcal{V} - C_2^\mathcal{V}\|_{C(I_\tau \times \bar{Q})} \leq c_3\tau^{1-\beta}\|\tilde{C}_1^\mathcal{V} - \tilde{C}_2^\mathcal{V}\|_{C(I_\tau \times \bar{Q})},$$

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  $\mathcal{L}: B_{\tau_0} \rightarrow B_{\tau_0}$  is a strict contraction and, thus, has a unique fixed point  $C^\mathcal{V} \in B_{\tau_0}$ .

The existence and regularity results 5.25, 5.26 and 5.40 prove that  $C^\mathcal{V}$  and the corresponding microscopic solution  $(\phi, c_s, v, p, u)$  solves the fully coupled two scale model and that in fact

$$C^\mathcal{V} \in C^1\left(I, (W_{r_2}^1(Q))'\right) \cap C\left(I, W_{r_2}^1(Q)\right).$$

Uniqueness follows as in the proof of Theorem 5.25. □



## 6 Summary

The thesis investigates a two scale model for liquid phase epitaxy, which also describes elastic effects. Liquid phase epitaxy is a technical process for the production of thin films and layers out of a liquid solution. The necessity of including elasticity into the model comes from the fact, that these effects have a significant impact on the development of the microstructure of the solid film, and the microstructure influences the physical properties of the layer.

Numerical simulations are of great importance from the scientific as well as from the commercial point of view. They allow to reproduce or even to predict the results of possibly expensive experiments. Thereby, the difficulty in liquid phase epitaxy is that a direct simulation has to resolve the microstructure, such that the simulation of a technically relevant device is almost impossible. The advantage of the two scale formulation is, that it opens up new possibilities for an efficient numerical simulation.

In order to validate the significance of a mathematical model, two aspects are of special interest: First, an analytical investigation can answer the question, if there even exists a solution of the model and if it is unique. If there is no solution, the model is useless and if it is not unique, the model is incomplete. Second, a solution should be computed numerically and the results should be compared to experiments. The thesis gives a positive answer to the first point and provides a basis for the handling of the second.

As main result of the thesis, existence and uniqueness of a solution is proven in suitable function spaces. Comparing the analogous result for the model without elasticity, the analysis here is much more demanding, with the Stokes problem posed in an unbounded domain and the free boundary in the microscopic cells, which makes the problem fully nonlinear. In the proof, the single problems (microscopic: Stokes, elasticity and phase field, macroscopic: convection-diffusion) are studied first, where the coupling data is supposed to be given. For each of them, the solvability is shown and furthermore it is proven, that the dependencies between each other are continuous. This allows the application of fixed point arguments: A first application of Banach' Fixed Point Theorem yields the existence and uniqueness of a solution for the coupled microscopic problem. A second treats the coupling between the microscopic and the macroscopic parts of the model and proves the main result.

The iterative procedure, which is proposed in chapter 4, relies on Banach's fixed point iterations. Its convergence is proven in this thesis. It is a basis for solving the problem numerically.

An interesting point for future work is the implementation of a numerical algorithm in order to compute a solution of the two scale model. The two scale formulation allows to use a coarse grid for the macroscopic model. The main difficulty to overcome is, that at each macroscopic grid point on the substrate a microscopic cell problem of high complexity has to be solved. This limits the possible size of the simulated layer.

A promising approach is the application of an adaptive solution strategy, where not every microscopic problem is solved, but only few selected. The microstructure at the other points can then be adapted from cells with "similar" macroscopic coupling data,

where the meaning of "similar" has to be specified by a suitable metric. Additionally, microscopic problems at different points can be computed in parallel, since they do not influence each other directly.

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.

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