Evolving Microstructure and Homogenization

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Abstract

In this article we formulate a mathematical model for the temporally evolving microstructure generated by phase changes and study the homogenization of this model. The investigations are partially formal, since we do not prove existence or convergence of solutions of the microstructure model to solutions of the homogenized problem. To model the microstructure, the sharp interface approach is used. The evolution of the interface is governed by an everywhere defined distribution partial differential equation for the characteristic function of one of the phases. This avoids the disadvantage commonly associated with this approach of an evolution equation only defined on the interface. To derive the homogenized problem, a family of solutions of the microstructure problem depending on the fast variable is introduced. The homogenized problem obtained contains a history functional, which is defined by the solution of a initial-boundary value problem in the representative volume element. In the special case of a temporally fixed microstructure the homogenized problem is reduced to an evolution equation to a monotone operator.

1 Introduction

Alloys used in jet engines display a microstructure, whose configuration evolves in time under loading. This microstructure, which is formed by phase changes of the material, influences the creep behavior of the alloy. A mathematical model describing the stress and deformation behavior of the alloy must therefore also account for the evolving microstructure. Since in this microstructure the length scale of the phase changes is less than $0.5\mu m$, effective numerical computations of the stress and strain fields in metallic components, whose dimensions lie in the range of centimeters or meters, can not be based on a

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microscopic mathematical model which faithfully describes the evolving microstructure. A macroscopic model is needed for this purpose. An interesting idea to develop a macroscopic model is to formulate a microscopic model first and then to derive a macroscopic model from it by homogenization. In this article we want to contribute to the development of this idea. We derive and formulate a microscopic model, which is of the sharp interface type, and study the homogenization of the partial differential equations in this model. The homogenized problem obtained contains a history functional, which is defined via the solution of an initial-boundary value problem in the representative volume element. The derivation of the homogenized equations is partly formal, since neither do we prove existence or uniqueness of solutions for the microscopic model, nor do we prove convergence of solutions of the microscopic model to solutions of the homogenized equations, assuming that such solutions exist. Such investigations must be left to later work. However, as a special case the model we derive describes microstructures, which do not evolve, but are temporally fixed. In this simpler case we discuss the homogenized initial-boundary value problem more precisely and verify some results towards an existence proof for solutions of this initial-boundary value problem.

To understand the mathematical investigations in this paper it is helpful to know the mechanical background of the mathematical model. Therefore we sketch this mechanical background first. Detailed descriptions and experimental and theoretical investigations can be found in [29, 18, 54, 67].

Nickel based single crystal alloys display a microstructure after production. For simplicity, we discuss alloys which only consist of the two components aluminium and nickel. Embedded in a matrix phase γ are cubic precipitates γ'. After complete aging the precipitates are distributed in the γ–matrix phase as a periodic array of cuboids of fairly uniform size. The length of the edges and the mutual distance of the precipitates is in the range of 0.2–$0.5\mu m$. The γ'–phase is highly ordered: The large aluminium atoms are placed in the crystal lattice at the eight corners of a cube and the nickel atoms are placed at the center of the six sides of this cube. In the γ–matrix phase the aluminium and the nickel atoms are distributed randomly over the positions in the crystal lattice. There is a mismatch between the lattice parameters a_γ and $a_{\gamma'}$ of the crystal in the γ– and γ'–phases. Typically the mismatch

$$\delta = \frac{a_{\gamma'} - a_\gamma}{a_\gamma}$$

is of the order of $|\delta| \leq 0.005$. Nevertheless, this small mismatch introduces a significant internal stress in the crystal at the phase interfaces and is considered to be the reason for the evolution of the morphology of the precipitates, which happens at high temperatures under the application of external stress. Two different types of evolution have been observed: Either the cuboids coarsen preferentially along the direction of the applied stress and form plates which lie parallel to the stress direction; or the coarsening is normal to the applied stress and plates form with the faces normal to the stress direction. The difference in the coarsening directions is attributed to the different crystal structures of the alloys.

As an important aspect, a mathematical model for this type of problem must account for the phase changes. Two approaches are used to model temporally evolving phase changes mathematically; both are employed in the different mathematical models, which have been developed to model the microstructure and the stress-strain behavior of single crystal alloys: In the *phase field approach* the different phases are characterized by an order parameter, which varies rapidely but smoothly and is assumed to satisfy a diffusion equation. The two phases are separated by the transition region of the order parameter. In the *sharp interface approach* the different phases are assumed to be separated by sharp moving interfaces. The movement of the interfaces is determined by an equation for the normal speed of the interfaces. The basic principle used in all investigations and models to govern the movement of the interfaces or the evolution of the order parameter is the second law of thermodynamics, which requires that this movement or evolution tend to decrease the free energy.

Mathematical models for the evolving microstructure in single crystal alloys using the phase field approach are formulated in [18, 78]; the sharp interface approach is used in [33, 55, 64, 65, 67], for example. Of these references, only [18] contains a complete set of model equations; in the others the main interest is to compute the equilibrium states of the microstructure. They do not give such a complete set of equations, which is not needed for this purpose.

In continuum mechanics and in the material sciences the investigation of moving interfaces and phase changes is a very active field of research with a long history. From the large body of literature we only mention [1, 5, 21, 22, 34, 35, 36, 47, 49, 50, 56]. Together with more articles several of these are collected in the book [6]. For detailed studies we must refer the reader to the bibliography contained in these articles.

From the mathematical literature about moving interfaces, moving boundaries and phase transitions we can only mention here [4, 8, 9, 10, 11, 13, 14, 17, 20, 27, 30, 31, 40, 48, 57, 68, 72, 73, 74, 76]. Many of the mathematical investigations concern interface problems, where the free energy has a nonvanishing surface part. This leads to problems of mean curvature flow or a generalization of it. Together with the constitutive assumption that the free energy is only a function of space, time and normal velocity of the interface, the problem can be reduced to the solution of a scalar partial differential equation, which in most cases is parabolic. An extensive theory also exists for the phase field approach, where the coupled evolution of the order parameter and the temperature field is studied. We refer in particular to [4]. This approach leads to initial-boundary value problems for a parabolic system or for a parabolic system coupled with other equations. In the recent investigation [30], the phase field approach is used to study temporally evolving phase changes in an elastic medium. Local existence of solutions is proved and the sharp interface limit is studied in the stationary case.

Concerning homogenization, we mention the articles [19, 46, 51, 53, 59, 60, 61, 62, 66, 69, 70], where the engineering view is dominating. A theoretical view predominates in the books and articles [3, 7, 12, 15, 24, 25, 37, 38, 39, 41, 42, 43, 44, 45, 52, 58, 63, 71]. The first group of articles contains investigations of the homogenization of problems with evolving microstructure as well as with temporally fixed microstructure, and numerical algorithms to compute the overall response of solids with microstructure. [12] and [58] from the second group discuss homogenization of nonlinear monotone operators, which is of interest for the investigations in Section 4. There the homogenization of initial-boundary value problems for inelastic materials with temporally fixed microstructure is studied, which, after a suitable transformation, can often be written as an evolution equation to a monotone operator. This is shown in [2]. In [52] the homogenization of a rate independent model for phase transformations is investigated. The homogenization of complicated time dependent flow problems from chemistry and engineering is discussed in [38, 39, 42]. The mathematical models studied in these articles contain transmission conditions and partial differential equations defined on the boundary manifold. In [15, 24, 25, 37] the homogenization of Hamilton-Jacobi equations is discussed in the frame of the theory of viscosity solutions.

We finally summarize the content of this article: In Section 2 we formulate a model for the evolving microstructure in single crystal alloys, which is of the sharp interface type. The basic, standard assumptions we use to formulate it are the same as in the model of Socrate and Parks [67]. In this model, the free energy does not have a surface part, but the material is allowed to show inelastic stress-strain behavior. This stress-strain behavior may be different in the two different phases. It is modeled using internal variables.

To characterize the two phases we introduce an order parameter which only takes the values 0 and 1 and thus jumps at the face interface. Using an order parameter is not new in the sharp interface approach, since the level set method uses such a parameter, for example. However, the choice of a discontinuous order parameter is in contrast both to the phase field approach and to the level set method, where the order parameters are smooth.

We first use the second law of thermodynamics to derive dissipation inequalities, which must be satisfied by the normal velocity of the phase interfaces and by the time derivative of the internal variables. These dissipation inequalities restrict the constitutive relations for the normal velocity and for the internal variables. The derivation is standard, but we present it for completeness and for definitness. As usual, it follows that the driving traction for the phase interface is generated by a jump of the Eshelby tensor at the interface; this jump is caused by the misfit strain originating from the different values of the lattice parameters in the γ– and γ'–phases. Since the free energy does not have a surface part, the mean curvature does not appear in the equations. We then formulate a constitutive equation for the normal velocity of the phase interfaces, which is in accordance with these restrictions. This equation can be considered to be an evolution equation for the phase interface. The mathematical model thus consists of an initial-boundary value problem to a system, which consists of partial differential equations for the strain and stress fields and of evolution equations for the internal variables and the phase interface. This model is derived in Sections 2.1 and 2.2.

Our new contributions to the modelling of moving phase interfaces are contained in Sections 2.3 to 2.5. A drawback of the sharp interface approach is that the equation for the normal speed of the interface is only defined on the interface, which causes difficulties in theoretical investigations and numerical computations. For example, the coalescence or the separation of precipitates will be difficult to model and to study. However, in a first step we show that the equation for the normal speed of the interface can be reformulated as an evolution equation for the discontinuous order parameter S taking the value 0 on the γ–phase and the value 1 on the γ'–phase. The evolution equation holds in the distribution sense and is defined everywhere, not only on the interfaces. Since knowledge of the interfaces is not needed to formulate the equation, the above mentioned drawback of the second approach is removed. Still, this equation is complicated and will not be easy to use. In a second step we therefore show that if the solution of this equation is smooth, it can be reduced to the first order partial differential equation

$$S_t(x,t) = -c\rho\psi_S(\varepsilon, S, z)\,|\nabla_x S(x,t)|$$

for S, a transport equation or Hamilton-Jacobi equation. Here ψ_S is the partial derivative of the free energy with respect to S, c is a constant and ρ, ε, z denote the density, the strain and the vector of internal variables. We surmise that the initial-boundary value problem with this equation as evolution equation for the order parameter has smooth solutions to smooth initial data, and that these smooth solutions can be used to approximate theoretically and numerically the discontinuous solutions to the original microstructure problem.

In Section 3 we formally derive the homogenized initial-boundary value problem associated to this microstructure model. The microstructure is introduced in the problem by assuming that the initial data for the order parameter are given by a function of the form

$$S^{(0)}(x, \frac{x}{\eta}),$$

where $y \to S^{(0)}(x,y)$ is periodic and where $\eta > 0$ is a small parameter. x is called the slow variable, y the fast variable. This means that the initial data are approximately periodic in space and that the scale of the microstructure tends to zero for $\eta \to 0$. To derive the homogenized equations, we assume that the microscopic initial-boundary value problem has solutions to these initial data with an order parameter of the form

$$S_\eta(x, \frac{x}{\eta}, t),$$

where $S_\eta(x,y,t)$ is periodic in the fast variable y and tends to $S_0(x,y,t)$ for $\eta \to 0$ in a suitable sense. Moreover, it is assumed that the other unknowns in the initial-boundary value problem have similar representations. By letting tend $\eta \to 0$, an initial-boundary value problem is determined which must be solved by S_0 and by the limit functions of the other unknowns. This is the homogenized problem. The homogenized problem consists of a macroscopic initial-boundary value problem in the macroscopic (x,t)–variables for the macroscopic deformation $u_0(x,t)$ and the macroscopic mean stress $T_\infty(x,t)$, with a history functional

$$T_\infty(x,t) = \mathcal{F}_{s \le t}(\nabla_x u_0(x,s)),$$

which for every x is computed via the solution of an initial-boundary value problem in the (y,t)–variables. y varies in the periodicity cell. This periodicity cell, or better, the initial-boundary value problem in the periodicity cell, is called representative volume element.

The evolution equation for the order parameter in the microscopic problem is a partial differential equation containing derivatives with respect to x and t. These derivatives are distribution derivatives. It turns out that in the initial-boundary value problem of the representative volume element the function $(y,t) \to S_0(x,y,t)$ must solve a partial differential equation containing distribution derivatives with respect to y and t. As usual in the theory of distributions, to define distribution derivatives with respect to y, an integration with respect to the y–variable must be present. To introduce this integration, we define in Section 3.1 the notion of *a family of solutions of the microscopic initial-boundary value problem depending on the fast variable* and generalize it in Section 3.4 to distribution solutions. For a precise discussion of the homogenized initial-boundary value problem we refer to the scholia after Definition 3.11 of this homogenized initial-boundary value problem in Section 3.4.

The reduction of the microscopic initial-boundary value problem to a homogenized problem with history functional defined via the solution of an initial-boundary value problem in the representative volume element is not completely satisfactory, since, as is discussed more precisely in the scholia after Definition 3.11, the determination of such a history functional still is of high computational complexity. Therefore this first homogenization should be followed in a second step by a homogenization of this representative volume element, which results in the elimination of the y–variable. Ideas have been developed for such a second homogenization, cf. [46, 52, 59, 60, 61, 62, 69, 70]. We can not discuss these ideas here, but have to refer to these articles and to the literature cited there.

In Section 4 we specialize the model to the simpler situation of a temporally fixed microstructure. In this simpler situation it is suggestive to interpret the homogenized initial-boundary value problem as a quasi-static problem with a constitutive equation, which is an ordinary differential equation in an infinite dimensional Banach space. We reduce the problem to an evolution equation and show that this is an evolution equation to a monotone operator, if the constitutive equation for the original microscopic problem is of monotone type. This is an important step towards an existence proof for solutions of the homogenized problem.

2 A mathematical model with sharp phase interfaces

2.1 Equations for the stress, displacement and internal variables

In this section we introduce the model equations for the stress, displacement and internal variables. These equations coincide essentially with the equations for homogeneous inelastic materials discussed in the book [2]. The only differences are that the microstructure introduces inhomogeneity in the material and that the equations used here contain a term representing the misfit strain. Therefore we only state these equations and refer the reader to [2] for a precise discussion. Also, we formulate interface conditions, boundary conditions and initial conditions.

To model phase changes evolving in time one needs in addition to the model equations for inelastic materials an evolution equation for the phase interfaces. Sections 2.2–2.5 are devoted to the formulation and transformation of this equation.

Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with smooth boundary $\partial\Omega$. It represents the points of a material body. By $\gamma(t)$ we denote the set of points of Ω, which at time t belong to the γ–phase, whereas $\gamma'(t)$ denotes the set of points of Ω which at time t belong to the γ'–phase. We assume that $\gamma(t)$ is closed in Ω and that

$$\gamma(t) \cap \gamma'(t) = \emptyset\,, \quad \gamma(t) \cup \gamma'(t) = \Omega\,.$$

The interface between the two phases is

$$\Gamma(t) = \gamma(t) \cap \overline{\gamma'(t)}.$$

These subsets of Ω are the cross sections at time t of the sets

$$\gamma = \{(x,t) \in \Omega \times \mathbb{R}_0^+ \mid x \in \gamma(t)\}, \quad \gamma' = \{(x,t) \in \Omega \times \mathbb{R}_0^+ \mid x \in \gamma'(t)\}$$

and

$$\Gamma = \{(x,t) \in \Omega \times \mathbb{R}_0^+ \mid x \in \Gamma(t)\}.$$

If in the following we do not mention special assumptions, we shall always assume that Γ is a sufficiently smooth submanifold of $\Omega \times \mathbb{R}_0^+$. To represent these sets, we introduce an order parameter $S : \Omega \times \mathbb{R}_0^+ \to \{0,\, 1\}$ with

$$S(x,t) = \begin{cases} 0\,, & x \in \gamma(t) \\ 1\,, & x \in \gamma'(t)\,. \end{cases}$$

Let $\mathcal{S}^3$ denote the set of symmetric 3×3–matrices, let $u : \Omega \times \mathbb{R}_0^+ \to \mathbb{R}^3$ denote the displacement and

$$\varepsilon\Big(\nabla_x u(x,t)\Big) = \frac{1}{2}\Big[\nabla_x u(x,t) + (\nabla_x u(x,t))^T\Big] \in \mathcal{S}^3$$

the linear strain tensor. Here $(\nabla_x u(x,t))^T$ denotes the transpose of the 3×3–matrix $\nabla_x u(x,t)$, the matrix of first order partial derivatives of u with respect to $x = (x_1, x_2, x_3)$. The function $T : \Omega \times \mathbb{R}_0^+ \to \mathcal{S}^3$ is the Cauchy stress tensor and $z : \Omega \times \mathbb{R}_0^+ \to \mathbb{R}^N$ is the vector of internal variables. Finally, $b : \Omega \times \mathbb{R}_0^+ \to \mathbb{R}^3$ is the given volume force. The strain and stress distributions are governed by the equations

$$
\begin{aligned}
-\mathrm{div}_x T(x,t) &= b(x,t) &(2.1)\\
T(x,t) &= D(S(x,t))\Big(\varepsilon(\nabla_x u(x,t)) - \varepsilon^*(S(x,t)) - Bz(x,t)\Big) &(2.2)\\
z_t(x,t) &= f(S(x,t),\, T(x,t),\, z(x,t))\,, &(2.3)
\end{aligned}
$$

which must be satisfied for all $t \geq 0$ and for all $x \in \Omega\backslash\Gamma(t)$. Here $D(0),\ D(1) : \mathcal{S}^3 \to \mathcal{S}^3$ are linear, symmetric, positiv definite mappings. $D(0)$ is the elasticity tensor in the matrix phase γ, and $D(1)$ is the elasticity tensor in the γ'–phase. $\varepsilon^*(1) \in \mathcal{S}^3$ is the misfit strain in the γ'–phase. The misfit strain is equal to zero in the matrix–phase, hence $\varepsilon^*(0) = 0$.

$B : \mathbb{R}^N \to \mathcal{S}^3$ is a linear mapping, which maps the vector of internal variables to the plastic strain tensor:

$$\varepsilon_p(x,t) = Bz(x,t)\,.$$

The given function $f : \Delta(f) \subseteq \{0,1\} \times \mathcal{S}^3 \times \mathbb{R}^N \to \mathbb{R}^N$ in the evolution equation (2.3) for the vector z of internal variables determines the inelastic properties of the γ– and γ'–phases of the material. Here $\Delta(f)$ denotes the domain of definition of f. This function depends on S, since the two phases behave differently. Purely elastic behavior in the γ'–phase is obtained with $f(1,\varepsilon,z) \equiv 0$.

On the interface $\Gamma(t)$ the functions $u,\ T$ and z must satisfy interface conditions. The functions $\varepsilon(\nabla_x u),\ u_t,\ T$, and z can jump across Γ, but we assume that the displacement u and the traction vector are continuous across the interface. Thus, with a given function $g : \mathbb{R}^N \to \mathbb{R}^N$ the interface conditions for $u,\ T$ and z are

$$
\begin{aligned}
u^+(x,t) &= u^-(x,t), &(2.4)\\
T^+(x,t)n(x,t) &= T^-(x,t)n(x,t), &(2.5)\\
z(x,t+) &= g(z(x,t-)), &(2.6)
\end{aligned}
$$

which must hold for all $(x,t) \in \Gamma$. Here $n(x,t) \in \mathbb{R}^3$ is the unit normal vector to $\Gamma(t)$ pointing from $\gamma'(t)$ to $\gamma(t)$. Also, $T^+(x,t)$ and $T^-(x,t)$ are the limit values of T if the argument tends to $(x,t) \in \Gamma$ from γ or from γ', respectively.

Precisely, for a function w and $(x,t) \in \Gamma$ we define

$$\begin{aligned} w^+(x,t) &= \lim_{\substack{\eta\to 0\\ \eta>0}} w((x,t)+\eta m(x,t)) \\ w^-(x,t) &= \lim_{\substack{\eta\to 0\\ \eta<0}} w((x,t)-\eta m(x,t)), \end{aligned}$$

with the unit normal vector $m(x,t) \in \mathbb{R}^4$ to Γ pointing from γ' to γ. In the following we assume that this normal vector differs everywhere from the vector $(0, \pm 1) \in \mathbb{R}^3 \times \mathbb{R}$.

Finally, the boundary condition is

$$T(x,t)n(x) = 0, \quad x \in \partial\Omega,\ t \geq 0, \tag{2.7}$$

with a unit vector $n(x)$ normal to $\partial\Omega$ at x, and the initial conditions are

$$z(x,0) = z^{(0)}(x), \quad S(x,0) = S^{(0)}(x), \quad x \in \Omega. \tag{2.8}$$

Under suitable regularity conditions for Γ and b, the equations (2.1) and (2.5), respectively, hold in the classical sense in $(\Omega \times \mathbb{R}^+)\backslash\Gamma$ and on Γ, respectively, if and only if T is a weak solution of (2.1) in $\Omega \times \mathbb{R}^+$. By definition, T is a weak solution if and only if

$$\int_0^\infty \int_\Omega T(x,t) : \nabla_x \varphi(x,t)\, dxdt = \int_0^\infty \int_\Omega b(x,t) \cdot \varphi(x,t)\, dxdt \tag{2.9}$$

is satisfied for every function $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^+, \mathbb{R}^3)$.

Remark. Instead of (2.6) we require in Section 3 that z is continuous across the interface Γ. We caution the reader that in this article v does not normally denote velocity. Instead, by v we denote functions with values in $\mathcal{S}^3$ or in $\mathbb{R}^m$ with $m \geq 1$.

2.2 Evolution equation for the phase interface, dissipation inequality

The $3 + 9 + N$ equations (2.1)–(2.3) contain the $3 + 9 + N + 1$ unknown components of u, T, z und S. Therefore the system (2.1)–(2.3) is not closed; an evolution equation for the order parameter S is missing. The evolution of S is known if and only if the evolution of the sets $\gamma(t)$ and $\gamma'(t)$ is known, and this evolution is known, if a constitutive equation is known, which determines the normal speed of the interface between the phases as a function of u, T and z. In this section we first derive restrictions for the form of such an equation from the second law of thermodynamics, essentially following the standard arguments in thermodynamics. Our presentation is influenced by

[35]. We then formulate a constitutive equation for the normal speed, which is in accordance with these restrictions. In Section 2.3 this equation is used to formulate an evolution equation for the order parameter S.

Let $\psi = \psi(\varepsilon, S, z)$ be the free energy. We assume that

$$\psi : \Delta(\psi) \to \mathbb{R}$$

is a sufficiently smooth function, whose domain of definition $\Delta(\psi)$ is equal to the set $\mathcal{S}^3 \times \{0,1\} \times \mathbb{R}^N$ or to a suitable subset of it. ψ must satisfy the basic equation

$$\rho \nabla_\varepsilon \psi(\varepsilon, S, z) = T\,, \tag{2.10}$$

(cf. [2]), where $\rho > 0$ denotes the mass density. In this article we assume that ρ is a constant. Insertion of (2.2) into (2.10) and integration yields

$$\rho\psi(\varepsilon, S, z) = \frac{1}{2}\Big[D(S)\Big(\varepsilon - \varepsilon^*(S) - Bz\Big)\Big] : \Big(\varepsilon - \varepsilon^*(S) - Bz\Big) + \psi_1(S, z),$$

with a suitable function ψ_1.

Second law of thermodynamics. We use the second law of thermodynamics in the following form: For every subregion R of Ω with sufficiently smooth boundary ∂R the displacement u, the stress T, the vector of internal variables z and the order parameter S must satisfy the inequality

$$\begin{aligned} \frac{d}{dt}\int_R \rho\psi(\varepsilon(\nabla_x u), S, z)\,dx \quad &\leq \quad \int_{\partial R} q(\varepsilon(\nabla_x u), u_t, S, z)\cdot n(x)\,d\sigma(x) \\ &\qquad + \int_R b\cdot u_t\,dx\,, \end{aligned} \tag{2.11}$$

with the negative energy flow (the stress power)

$$q(\varepsilon(\nabla_x u), u_t, S, z) = T(\varepsilon(\nabla_x u), S, z)u_t\,.$$

Here $n(x)$ is a unit vector normal to ∂R pointing out of R.

Theorem 2.1 (Dissipation inequalities for the internal variables and for the phase boundary) *Let $(u, T, z, S) : \Omega \times \mathbb{R}_0^+ \to \mathbb{R}^3 \times \mathcal{S}^3 \times \mathbb{R}^N \times \{0,1\}$ be a function, which is continuously differentiable on the closed set γ and on the set γ', and which is such that $(u,T,z,S)\big|_{\gamma'}$ has a continuously differentiable extension to $\overline{\gamma'}$.*

(i) *Then (2.11), the second law of thermodynamics, implies*

$$\rho\frac{\partial}{\partial t}\psi(\varepsilon, S, z) - \operatorname{div}_x q(\varepsilon, u_t, S, z) - b\cdot u_t \leq 0 \tag{2.12}$$

on $\Omega \times \mathbb{R}^+$ in the weak sense.

(ii) *Assume in addition that* u, T, z, S *satisfy* (2.1), (2.2) *on* $\Omega \times \mathbb{R}^+$ *and* (2.4) (2.5) *on the phase interface* Γ. *Then* (2.12) *holds if and only if the following two inequalities are satisfied:*

$$\rho \nabla_z \psi(\varepsilon(\nabla_x u(x,t)), S(x,t), z(x,t)) \cdot z_t(x,t) \le 0 \tag{2.13}$$

for almost all $(x,t) \in \Omega \times \mathbb{R}_0^+$, *and*

$$m''(x,t)\Big(m'(x,t) \cdot \Big[C\Big(\nabla_x u(x,t), S(x,t), z(x,t)\Big)\Big] m'(x,t)\Big) \le 0 \tag{2.14}$$

for all $(x,t) \in \Gamma$. *Here* $m(x,t) = (m'(x,t), m''(x,t)) \in \mathbb{R}^3 \times \mathbb{R}$ *is a unit normal vector to* Γ *pointing from* γ' *to* γ ,

$$\begin{aligned} C(\nabla_x u, S, z) &= \rho\psi(\varepsilon(\nabla_x u), S, z) I - (\nabla_x u)^T T \\ &= \rho\psi(\varepsilon(\nabla_x u), S, z) I - (\nabla_x u)^T (D(S)(\varepsilon(\nabla_x u) - \varepsilon^*(S) - Bz)) \end{aligned} \tag{2.15}$$

is the Eshelby tensor, and

$$[C] = C^+ - C^-$$

denotes the jump of C *along the phase boundary* Γ . *By* I *we denote the unit matrix.*

Remark. By definition, (2.12) is satisfied in the weak sense if

$$\int_{\Omega \times \mathbb{R}^+} \Big(- \rho\psi(\varepsilon, S, z)\varphi_t + q(\varepsilon, u_t, S, z) \cdot \nabla_x \varphi - b \cdot u_t \varphi \Big) \, d(x,t) \le 0$$

for all $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^+, \mathbb{R})$ with $\varphi(x,t) \ge 0$.

Since we assumed that $m(x,t) \ne (0, \pm 1)$, hence $m'(x,t) \ne 0$, it follows that (2.14) is equivalent to

$$\nu\Big(n \cdot \Big[C(\nabla_x u, S, z)\Big] n\Big) \ge 0 \, ,$$

with the unit normal vector $n = \frac{m'}{|m'|} \in \mathbb{R}^3$ to $\Gamma(t)$ and with

$$\nu(x,t) = -\frac{m''(x,t)}{|m'(x,t)|} \, . \tag{2.16}$$

$\nu(x,t)$ is the normal speed of propagation of the phase interface $\Gamma(t)$ at the point x in the direction of $n(x,t)$. Therefore we have the following

Corollary 2.2 (Constitutive equation for the normal speed of the phase interface.) *Let $c : \mathbb{R} \to \mathbb{R}$ be a given function with $c(s)s \geq 0$ for all $s \in \mathbb{R}$. If u, T, z, S satisfy* (2.1)–(2.5)*, if the normal speed of the phase interface satisfies*

$$\nu(x,t) = c\Big(n(x,t) \cdot \Big[C\Big(\nabla_x u(x,t), S(x,t), z(x,t)\Big)\Big] n(x,t)\Big) \tag{2.17}$$

for all $(x,t) \in \Gamma$, and if the dissipation inequality

$$\rho \nabla_z \psi(\varepsilon, S, z) \cdot f(S,T,z) \leq 0 \tag{2.18}$$

is satisfied for all

$$(\varepsilon, S, z) \in \Delta(\psi) \cap \{(\varepsilon, S, z) \mid (S,T,z) \in \Delta(f)\},$$

then the inequality (2.12) *expressing the second law of thermodynamics is fulfilled.*

Remark. Since by assumption (2.2) is satisfied, we consider here $T = T(\varepsilon, S, z)$ to be a function of (ε, S, z). (2.18) is the well known dissipation inequality for constitutive equations with internal variables, cf. [2].

Proof of the Corollary: The equation (2.17) implies (2.14), and (2.13) is implied by (2.3) and (2.18). Therefore the statement follows from Theorem 2.1.

Proof of Theorem 2.1: (i) Assume that the inequality (2.11) holds. To every function $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^+)$ satisfying $\varphi(y,t) \geq 0$ for all $(y,t) \in \Omega \times \mathbb{R}^+$ we can choose a number $r \in \mathbb{R}$ such that

$$0 < r < \frac{1}{2} \operatorname{dist}\Big(\operatorname{supp}\varphi,\ \partial(\Omega \times \mathbb{R}^+)\Big).$$

Then for every $(y,t) \in \operatorname{supp}\varphi$ the closed ball

$$\overline{B_r(y)} = \{x \in \mathbb{R}^3 \mid |x - y| \leq r\}$$

belongs to Ω. In (2.11) we choose $R = B_r(y)$ with $(y,t) \in \Omega \times \mathbb{R}^+$, multiply the inequality with $\varphi(y,t)$ and integrate with respect to (y,t). The result is

$$\begin{aligned}
&\int_{\Omega \times \mathbb{R}^+} \varphi(y,t) \frac{d}{dt} \int_{|x-y|<r} \rho\psi(x,t)\, dx\, d(y,t) \\
&\quad \leq \int_{\Omega \times \mathbb{R}^+} \varphi(y,t) \int_{|x-y|=r} q(x,t) \cdot \frac{x-y}{r}\, d\sigma(x) d(y,t) \\
&\quad + \int_{\Omega \times \mathbb{R}^+} \varphi(y,t) \int_{|x-y|<r} (b \cdot u_t)(x,t)\, dx d(y,t),
\end{aligned}$$

where we used the notations

$$\psi(x,t) = \psi\Big(\varepsilon(\nabla_x u(x,t)), S(x,t), z(x,t)\Big)$$

and

$$q(x,t) = q\Big(\varepsilon(\nabla_x u(x,t)), u_t(x,t), S(x,t), z(x,t)\Big) .$$

Partial integration and interchange of the order of integration yields

$$\begin{aligned}
& -\int_{\Omega\times\mathbb{R}^+}\int_{|y-x|<r} \varphi_t(y,t)\rho\psi(x,t)\,dy\,d(x,t) \\
\leq \;& -\int_{\Omega\times\mathbb{R}^+}\int_{|y-x|=r} \varphi(y,t)\frac{y-x}{r}\,d\sigma(y)\cdot q(x,t)\,d(x,t) \\
& + \int_{\Omega\times\mathbb{R}^+}\int_{|y-x|<r} \varphi(y,t)(b\cdot u_t)(x,t)\,dy\,d(x,t) .
\end{aligned}$$

In the first term on the right hand side of this inequality we use the Divergence Theorem to obtain

$$\begin{aligned}
\int_{\Omega\times\mathbb{R}^+}\int_{|y-x|<r} \Big(& -\varphi_t(y,t)\rho\psi(x,t) + \nabla_y\varphi(y,t)\cdot q(x,t) \\
& - \varphi(y,t)(b\cdot u_t)(x,t)\Big)\,dyd(x,t) \leq 0 .
\end{aligned}$$

Since

$$\lim_{r\to 0}\frac{3}{4\pi r^3}\int_{|y-x|<r} \nabla_{(y,t)}\varphi(y,t)dy = \nabla_{(x,t)}\varphi(x,t) ,$$

uniformly with respect to $(x,t)\in\Omega\times\mathbb{R}^+$, we conclude from the last inequality that

$$\begin{aligned}
\int_{\Omega\times\mathbb{R}^+} \Big(& -\rho\psi(x,t)\varphi_t(x,t) + q(x,t)\cdot\nabla_x\varphi(x,t) \\
& - (b\cdot u_t)(x,t)\,\varphi(x,t)\Big)d(x,t) \leq 0
\end{aligned} \tag{2.19}$$

for all non-negative $\varphi\in C_0^\infty(\Omega\times\mathbb{R}^+)$. This proves (i).

(ii) Since S is constant on the sets γ and γ', it follows that on $\mathring{\gamma}$ and on γ' ,

$$\frac{\partial}{\partial t}\psi(x,t) = \nabla_\varepsilon\psi(\varepsilon,S,z) : \varepsilon_t + \nabla_z\psi(\varepsilon,S,z)\cdot z_t .$$

Therefore the inequality (2.19) is equivalent to

$$\begin{aligned}
\int_{\Omega\times\mathbb{R}^+} & \Big(\rho\nabla_\varepsilon\psi(\varepsilon,S,z) : \varepsilon_t + \rho\nabla_z\psi(\varepsilon,S,z)\cdot z_t \\
& - \operatorname{div}_x q(\varepsilon,u_t,S,z) - b\cdot u_t\Big)\varphi(x,t)d(x,t) \\
& + \int_\Gamma \Big(\rho[\psi(\varepsilon,S,z)]m'' - [q(\varepsilon,u_t,S,z)]\cdot m'\Big)\varphi(x,t)\,d\sigma(x,t) \leq 0 ,
\end{aligned}$$

where, as above, $m(x,t) = (m', m'') \in \mathbb{R}^3 \times \mathbb{R}$ is a unit normal vector to Γ pointing from γ' to γ and $[\psi] = \psi^+ - \psi^-$, $[q] = q^+ - q^-$ denote the jumps of ψ and q along Γ. Using that

$$\begin{aligned} \operatorname{div}_x q &= \operatorname{div}_x(Tu_t) = (\operatorname{div}_x T^T) \cdot u_t + T^T : \nabla_x u_t \\ &= (\operatorname{div}_x T) \cdot u_t + \rho(\nabla_\varepsilon \psi) : \varepsilon_t \,, \end{aligned} \tag{2.20}$$

where we employed (2.10) and the symmetry of T, the above inequality is seen to be equivalent to

$$\int_{\Omega\times\mathbb{R}^+} \Big(\rho \nabla_z \psi(\varepsilon, S, z) \cdot z_t - (\operatorname{div}_x T) \cdot u_t - b \cdot u_t\Big) \varphi(x,t)\, d(x,t) \\ + \int_\Gamma \Big(\rho[\psi] m'' - [Tu_t] \cdot m'\Big) \varphi(x,t)\, d\sigma(x,t) \leq 0\,.$$

Because of $\operatorname{div}_x T + b = 0$ and because of

$$[Tu_t] = \langle T\rangle [u_t] + [T]\langle u_t\rangle$$

with

$$\langle T\rangle = \frac{1}{2}(T^+ + T^-), \;\; \langle u_t\rangle = \frac{1}{2}(u_t^+ + u_t^-)\,,$$

this is equivalent to

$$\int_{\Omega\times\mathbb{R}^+} \Big(\rho \nabla_z \psi(\varepsilon, S, z) \cdot z_t\Big) \varphi(x,t) d(x,t) \\ + \int_\Gamma \Big(\rho[\psi] m'' - (\langle T\rangle m') \cdot [u_t] - ([T]m') \cdot \langle u_t\rangle\Big) \varphi(x,t)\, d\sigma(x,t) \leq 0\,. \tag{2.21}$$

Since $m' \in \mathbb{R}^3$ is normal to $\Gamma(t)$, it follows from (2.5) that $[T]m' = 0$. The vector field

$$(m'' m', -|m'|^2)$$

is tangential to Γ. Since by assumption u is continuously differentiable on $\overline{\gamma}$ and on $\overline{\gamma'}$ and continuous across Γ, it follows that the limits $(u_t)^\pm, (\nabla_x u)^\pm$ on Γ exist and that the tangential derivatives on both sides of Γ coincide:

$$-|m'|^2 u_t^+ + m''(\nabla_x u)^+ m' = -|m'|^2 u_t^- + m''(\nabla_x u)^- m'\,,$$

hence

$$[u_t] = [\nabla_x u] m' \frac{m''}{|m'|^2}\,.$$

Therefore (2.21) is equivalent to

$$\int_{\Omega\times\mathbb{R}^+} \Big(\rho \nabla_z \psi(\varepsilon, S, z) \cdot z_t\Big) \varphi(x,t) d(x,t) \\ + \int_\Gamma \Big(\rho[\psi] - \Big(\langle T\rangle \frac{m'}{|m'|}\Big) \cdot \Big([\nabla_x u] \frac{m'}{|m'|}\Big)\Big) m'' \varphi(x,t) d\sigma(x,t) \leq 0\,.$$

This inequality holds for all $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^+)$ with $\varphi \geq 0$ if and only if

$$\rho \nabla_z \psi(\varepsilon, S, z) \cdot z_t \leq 0$$

almost everywhere in $\Omega \times \mathbb{R}^+$ and

$$\Big(\rho[\psi] - \Big(\langle T \rangle \frac{m'}{|m'|}\Big) \cdot \Big([\nabla_x u] \frac{m'}{|m'|}\Big)\Big) m'' \leq 0 \qquad (2.22)$$

almost everywhere on Γ. We use again that $[T]m' = 0$, which implies

$$[\nabla_x u]^T \langle T \rangle m' = [\nabla_x u]^T \langle T \rangle m' + \langle \nabla_x u \rangle^T [T] m' = [(\nabla_x u)^T T] m',$$

whence (2.22) is equivalent to

$$\frac{m'}{|m'|} \cdot (\rho[\psi] I - [(\nabla_x u)^T T]) \frac{m'}{|m'|} m'' \leq 0 \quad \text{on } \Gamma.$$

This inequality can be written in the form (2.14) using the definition of the Eshelby tensor C in (2.15). The theorem is proven.

2.3 Evolution equation for the order parameter S

The equations (2.1)–(2.3), (2.17) form a closed system, since the evolution in time of the phase interface Γ can be determined from the normal velocity ν given in (2.17). However, instead of the equation (2.17) for the normal speed of the phase interface Γ one would prefer to have an evolution equation for the order parameter S directly. To derive such an equation we start from the method of characteristics, a customary way to model moving phase interfaces, cf. Taylor, Cahn and Handwerker [73]. The method is based on a partial differential equation readily derived from (2.16). We shortly sketch the iteration procedure which must be used to determine the manifold Γ with this method. After this we shall not follow this method any further; instead, we show that this partial differential equation can be used directly as an evolution equation for the order parameter S. This evolution equation is however a distribution equation.

Assume that Γ is a sufficiently smooth 3–dimensional submanifold of $\Omega \times \mathbb{R}^+$, that (m', m'') is a unit normal vector field on Γ, and that $\nu : \Gamma \to \mathbb{R}$ is the normal velocity of Γ. Then ν satisfies the equation (2.16) on all of Γ :

$$\nu(x,t) = -\frac{m''(x,t)}{|m'(x,t)|}\,.$$

Assume moreover that Γ is given by

$$\Gamma = \Big\{(x,t) \in \Omega \times \mathbb{R}^+ \,\Big|\, \chi(x,t) = 0\Big\}\,, \qquad (2.23)$$

with a suitable function χ. Then for all $(x,t) \in \Gamma$ the vector $(\nabla_x \chi(x,t), \chi_t(x,t))$ is normal to Γ, and we assume that it has the direction of $-(m'(x,t), m''(x,t))$, hence

$$(\nabla_x \chi, \chi_t) = -|(\nabla_x \chi, \chi_t)|\,(m', m'')\,.$$

From this equation and from (2.16) we infer that the equation

$$\chi_t(x,t) - \nu(x,t)|\nabla_x \chi(x,t)| = 0 \tag{2.24}$$

holds for all $(x,t) \in \Gamma$.

Conversely, if χ is a sufficiently smooth function which satisfies (2.24) and which on a 2–dimensional submanifold $\tilde{\Gamma}$ of Γ fulfills the initial condition

$$\chi(x,t) = 0, \quad (x,t) \in \tilde{\Gamma},$$

then χ vanishes on all of Γ, whence (2.23) is satisfied. This follows from the classical theory of first order partial differential equations. If for $(\xi, \zeta) \in \mathbb{R}^3 \times \mathbb{R}$ we set

$$p(x,t;\xi,\zeta) = \zeta - \nu(x,t)|\xi|\,,$$

then the equation (2.24) can be written in the form

$$p(x,t,\nabla_x \chi(x,t), \chi_t(x,t)) = 0\,.$$

However, the solution χ of this differential equation can not be determined in the usual manner by solving the characteristic system of ordinary differential equations, since $\nu(x,t)$ and $p(x,t;\xi,\zeta)$ are only defined for points (x,t) on the manifold Γ. The partial derivatives p_t and $\nabla_x p$ are therefore not defined. To solve the characteristic system it is necessary to extend ν smoothly from Γ to an open neighborhood of Γ by a suitable method. Then a solution of (2.24) can be obtained by solving the characteristic system

$$\begin{aligned}
\frac{dx}{ds} &= \nabla_\xi\, p(x,t;\xi,\zeta) \\
\frac{dt}{ds} &= \frac{\partial}{\partial \zeta}\, p(x,t;\xi,\zeta) \\
\frac{d\xi}{ds} &= -\nabla_x\, p(x,t;\xi,\zeta) \\
\frac{d\zeta}{ds} &= -\frac{\partial}{\partial t}\, p(x,t;\xi,\zeta)\,.
\end{aligned}$$

The solution χ of (2.24) is constant along the characteristic curves $s \mapsto (x(s), t(s))$, whence the manifold $\{\chi(x,t) = 0\}$ is generated by those characteristic curves $s \mapsto (x(s), t(s))$, which pass through $\tilde{\Gamma}$. That (2.23) holds can be deduced from (2.24), which implies that the normal vector field $(\tilde{m}', \tilde{m}'') = -(\nabla_x \chi, \chi_t)$ to the manifold $\chi(x,t) = 0$ satisfies

$$\nu(x,t) = -\frac{\tilde{m}''(x,t)}{|\tilde{m}'(x,t)|}\,.$$

Therefore, since the manifolds Γ and $\{\chi(x,t) = 0\}$ both contain $\tilde{\Gamma}$ as a submanifold and since the normal speeds coincide, it follows that $\Gamma = \{\chi(x,t) = 0\}$.

In these considerations we assumed that Γ and the normal velocity $\nu : \Gamma \to \mathbb{R}$ are known from the outset. However, in the initial-boundary value problem to the equations (2.1)–(2.3), (2.17) the unknowns are u, T, z and Γ. The normal speed is determined by (2.17) as a function of (u, T, z, Γ) and is also unknown. To determine these unknowns, we must use an iteration procedure: Start with an approximate phase interface Γ_0, determine to this approximate interface a solution (u, T, z) of the partial differential equations (2.1)–(2.3) with suitable boundary and initial conditions and with suitable interface conditions on Γ_0, and insert this solution into (2.17) to compute an approximate normal speed ν_0 on Γ_0. Insert ν_0 for ν into (2.24). After smooth extension of ν_0, a new approximate phase interface Γ_1 can be computed by solving this partial differential equation with the method of characteristics. The iteration can then be continued and one expects that the sequence of phase interfaces $\{\Gamma_0, \Gamma_1, \ldots\}$ tends to the correct interface sought.

We will not pursue this method further; instead, in the next lemma we show that without extending ν smoothly, the order parameter S can be inserted for χ in (2.24) directly. If ν is continued by zero from the manifold Γ to $\Omega \times \mathbb{R}^+$, then (2.24) can be interpreted as a partial differential equation, which holds on all of $\Omega \times \mathbb{R}^+$ in the sense of measures. This yields an evolution equation for S.

To formulate this result, we need the space $BV^{\mathrm{loc}}(\Omega \times \mathbb{R}^+)$ of functions in $L^{1,\mathrm{loc}}(\Omega \times \mathbb{R}^+)$, whose weak first derivatives are Radon measures. More precisely, a function h belongs to the space $BV^{\mathrm{loc}}(\Omega \times \mathbb{R}^+, \mathbb{R})$ if $h \in L^{1,\mathrm{loc}}(\Omega \times \mathbb{R}^+, \mathbb{R})$ and if for any open subset V compactly contained in $\Omega \times \mathbb{R}^+$

$$\sup\Big\{ \int_V h(x,t)\,\mathrm{div}\,\varphi(x,t)\,d(x,t) \;\Big|\; \varphi \in C_0^1(V, \mathbb{R}^4),\ |\varphi| \le 1 \Big\} < \infty.$$

Here $C_0^1(\Omega \times \mathbb{R}^+)$ denotes the space of all continuous mappings with compact support in $\Omega \times \mathbb{R}^+$. A function belonging to the space $BV^{\mathrm{loc}}(\Omega \times \mathbb{R}^+)$ is said to have locally bounded variation.

The derivatives h_t and h_{x_i} are signed measures. To these measures the total variation measures $|h_t|$ and $|\nabla_x h|$ can be introduced: For a measure μ on an open subset U and a measureable subset R of U the total variation measure

$|\mu|$ is defined by

$$|\mu(R)| = \sup \sum_{i=1}^{n} |\mu(R_i)| \,, \tag{2.25}$$

where the supremum is taken over all finite collections $\{R_i\}$ of μ–measurable, pairwise disjoint sets with $R_i \subseteq R$.

The set γ' is said to be of locally finite perimeter if the characteristic function S of this set belongs to the space $BV^{\text{loc}}(\Omega \times \mathbb{R}^+, \mathbb{R})$. In this case a unit normal vector field (m', m'') pointing from γ' to γ can be defined on the measure theoretic boundary $\Gamma_* \subseteq \Gamma$, which consists of all points $(x,t) \in \Gamma$ with

$$\limsup_{r\to 0} \frac{1}{r^4} |B_r(x,t) \cap \gamma'| > 0, \quad \limsup_{r\to 0} \frac{1}{r^4} |B_r(x,t) \backslash \gamma'| > 0.$$

Here $B_r(x,t) \subseteq \mathbb{R}^4$ is the ball with center (x,t) and radius r and $|\cdot|$ denotes the Lebesgue measure. For these and other results about the spaces BV^{loc} we refer to [26, 77, 75].

Lemma 2.3 *Assume that γ' is of locally finite perimeter with a unit normal vector field (m', m'') of Γ_* pointing from γ' to γ. Let $\nu : \Omega \times \mathbb{R}^+ \to \mathbb{R}$ be a function satisfying*

$$\nu(x,t) = 0, \quad (x,t) \in (\Omega \times \mathbb{R}^+) \backslash \Gamma_* \,.$$

Then S solves the equation

$$S_t = \nu \, |\nabla_x S| \tag{2.26}$$

if and only if

$$\nu(x,t) = -\frac{m''(x,t)}{|m'(x,t)|}$$

for σ_3–all $(x,t) \in \Gamma_*$, where σ_3 denotes the three dimensional Hausdorff measure.

Scholium. Because of $S \in BV^{\text{loc}}(\Omega \times \mathbb{R}^+)$, both members of the equation (2.26) are measures, and equality is meant in the sense of measures. The measures S_t and $\nabla_x S$ satisfy $S_t(V) = \nabla_x S(V) = 0$ for every open subset $V \subseteq (\Omega \times \mathbb{R}^+) \backslash \Gamma$, and the product $\nu |\nabla_x S|$ is the measure corresponding to the bounded linear form on $C_0(\Omega \times \mathbb{R}^+)$ defined by the integral

$$\varphi \mapsto (\nu |\nabla_x S|, \varphi) = \int_{\Omega \times \mathbb{R}^+} \varphi(x,t) \nu(x,t) \, d|\nabla_x S(x,t)| \,,$$

for $\varphi \in C_0(\Omega \times \mathbb{R}^+)$.

S must satisfy (2.26) with the normal speed of the phase boundary Γ given by (2.17) inserted for ν. Therefore (2.26) is the evolution equation for S. In the proof of Theorem 2.5 we also need the other direction of the statement of the lemma: If S is the characteristic function of the set γ' and satisfies an equation of the form (2.26), then ν must necessarily be the normal speed of the boundary Γ, along which S jumps.

Proof of Lemma 2.3: By definition of the distribution S_t and by the Divergence Theorem for functions of locally bounded variation (cf. [26, p. 209]), we obtain for $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^+)$

$$\begin{aligned}\int_{\Omega\times\mathbb{R}^+} \varphi(x,t)\, dS_t(x,t) &= -\int_{\Omega\times\mathbb{R}^+} \varphi_t(x,t) S(x,t)\, d(x,t) \\ = -\int_{\gamma'} \varphi_t(x,t)\, d(x,t) &= -\int_{\Gamma_*} m''(x,t)\varphi(x,t)\, d\sigma_3(x,t).\end{aligned}$$

For the measure S_t this means that

$$S_t = -m''\sigma_3\lfloor\Gamma_*\,, \tag{2.27}$$

where $\sigma_3\lfloor\Gamma_*$ denotes the restriction of the Hausdorff measure σ_3 to Γ_*. Similarly,

$$\begin{aligned}\int_{\Omega\times\mathbb{R}^+} \varphi(x,t)\, dS_{x_i}(x,t) &= -\int_{\Omega\times\mathbb{R}^+} \varphi_{x_i}(x,t) S(x,t)\, d(x,t) \\ &= -\int_{\Gamma_*} m_i'(x,t)\varphi(x,t)\, d\sigma_3(x,t)\,,\end{aligned}$$

hence $\nabla_x S = -m'\sigma_3\lfloor\Gamma_*$. This equation together with (2.25) implies

$$|\nabla_x S| = |m'|\sigma_3\lfloor\Gamma_*\,.$$

From this equation and from (2.27) we infer that $S_t = \nu\,|\nabla_x S|$ is equivalent to

$$-m''\sigma_3\lfloor\Gamma_* = \nu|m'|\sigma_3\lfloor\Gamma_*\,,$$

which holds if and only if $-m''(x,t) = \nu(x,t)|m'(x,t)|$ for σ_3–all $(x,t) \in \Gamma_*$. This completes the proof.

2.4 Weak form of the evolution equation for S

With the result of Lemma 2.3 we obtain an evolution equation for S by insertion of (2.17) into (2.26). Combination of the resulting equation with (2.1)–(2.3) yields a closed system for the unknown function (u, T, z, S). This system is

$$
\begin{aligned}
-\mathrm{div}_x T(x,t) &= b(x,t) && (2.28)\\
T(x,t) &= D(S(x,t))\Big(\varepsilon(\nabla_x u(x,t)) - \varepsilon^*(S(x,t)) - Bz(x,t)\Big) && (2.29)\\
z_t(x,t) &= f(S(x,t), T(x,t), z(x,t)) && (2.30)\\
S_t(x,t) & && (2.31)\\
&= c\Big(n(x,t)\cdot[C(\nabla_x u(x,t), S(x,t), z(x,t))]n(x,t)\Big)|\nabla_x S(x,t)|.
\end{aligned}
$$

In (2.31), $n(x,t)$ is a normal vector to the surface $\Gamma(t)$, which bounds the set $\gamma' = \{x \in \Omega \mid S(x,t) = 1\}$. Such a normal vector field can be defined if S belongs to the space $BV^{\mathrm{loc}}(\Omega \times \mathbb{R}^+)$. However, for several reasons it is advantageous to have an evolution equation without normal vectors. In this section we transform the evolution equation (2.31) into a form without normal vectors under the assumption, that the function c is linear. In Section 2.5 it is shown that this form of the evolution equation can be considerably simplified provided that the solutions are smooth. This is one of the advantages of the form without normal vectors.

Thus, in the remainder of this article c denotes a positive constant.

Lemma 2.4 *Assume that $(u,T,z,S) : \Omega \times \mathbb{R}_0^+ \to \mathbb{R}^3 \times \mathcal{S}^3 \times \mathbb{R}^N \times \{0,1\}$ satisfies the assumptions of Theorem 2.1 (ii). Then the following assertions hold:*

(i) *The equation*

$$|n \cdot [C]n| = |[C]n| \tag{2.32}$$

is satisfied on Γ, where $n(x,t) \in \mathbb{R}^3$ is a unit normal vector to $\Gamma(t)$ at $x \in \Gamma(t)$.

(ii) *Let the distribution $[C]n\,|\nabla_x S|$ be defined by*

$$\Big([C]n\,|\nabla_x S|, \varphi\Big) = \int_{\Omega\times\mathbb{R}^+} [C(x,t)]n(x,t)\varphi(x,t)\,d|\nabla_x S(x,t)|\,,$$

for $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^+, \mathbb{R}^3)$, with

$$[C(x,t)] = \begin{cases} [C(\nabla_x u(x,t), S(x,t), z(x,t))]\,, & (x,t) \in \Gamma \\ 0\,, & (x,t) \in (\Omega \times \mathbb{R}^+)\backslash\Gamma\,. \end{cases}$$

Then, in the sense of distributions,

$$
\begin{aligned}
\mathrm{div}_x\, C(\nabla_x u, S, z) - \rho(\nabla_x z)^T \nabla_z\, \psi(\varepsilon, S, z) - (\nabla_x u)^T b& \\
= [C]n|\nabla_x S|\,.&
\end{aligned} \tag{2.33}
$$

Remark. Precisely, (2.33) means that

$$
\begin{aligned}
&-\int_{\Omega\times\mathbb{R}^+} C(\nabla_x u, S, z) : \nabla_x \varphi \, d(x,t) \\
&\qquad -\int_{(\Omega\times\mathbb{R}^+)\backslash\Gamma} \Big(\rho(\nabla_x z)^T \nabla_z \psi(\varepsilon, S, z) + (\nabla_x u)^T b\Big) \cdot \varphi \, d(x,t) \\
&= \Big([C]n|\nabla_x S|, \varphi\Big)
\end{aligned}
$$

for all $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^+, \mathbb{R}^3)$. The derivatives of $\nabla_x z$ of z in (2.33) are the classical derivatives on $(\Omega \times \mathbb{R}^+)\backslash\Gamma$, not the distributional derivatives of z on $\Omega \times \mathbb{R}^+$. The function z can jump across Γ, in which case the distributional derivatives on $\Omega \times \mathbb{R}^+$ differ from the classical derivatives on $(\Omega \times \mathbb{R}^+)\backslash\Gamma$ by a measure on Γ. This measure does not appear in (2.33).

Proof: (i) The interface condition (2.5) yields $[T(x,t)]n(x,t) = 0$ for $(x,t) \in \Gamma$. (2.15) and the equation $[(\nabla_x u)^T T] = [(\nabla_x u)^T]\langle T\rangle + \langle(\nabla_x u)^T\rangle[T]$ thus imply

$$
\begin{aligned}
n \cdot [C]n &= n \cdot \Big(\rho[\psi] - [(\nabla_x u)^T T]\Big)n \qquad (2.34)\\
&= n \cdot \Big(\rho[\psi]n - [(\nabla_x u)^T]\langle T\rangle n - \langle(\nabla_x u)^T\rangle[T]n\Big) \\
&= n \cdot \Big(\rho[\psi]n - [\nabla_x u]^T\langle T\rangle n\Big).
\end{aligned}
$$

We now show that the range of the linear mapping $[\nabla_x u]^T$ is contained in the subspace of $\mathbb{R}^3$ spanned by $n(x,t)$. Since $\rho[\psi]$ is a scalar, statement (i) is an obvious consequence of this result and of (2.34).

Thus, assume that $\tau \in \mathbb{R}^3$ is orthogonal to $n \in \mathbb{R}^3$. Then τ is a tangential vector to $\Gamma(t)$. Since by assumption u is continuously differentiable on $\overline{\gamma(t)}$ and on $\overline{\gamma'(t)}$ and continuous across $\Gamma(t)$, it follows that the limits $(\nabla_x u)^\pm$ exist on $\Gamma(t)$ and that the tangential derivatives on both sides of $\Gamma(t)$ coincide. For every $v \in \mathbb{R}^3$ we thus obtain

$$
\begin{aligned}
\tau \cdot \Big([\nabla_x u]^T v\Big) &= \Big([\nabla_x u]\tau\Big) \cdot v \\
&= \Big(\Big((\nabla_x u)\tau\Big)^+ - \Big((\nabla_x u)\tau\Big)^-\Big) \cdot v \\
&= \Big(\Big(\frac{\partial}{\partial\tau} u\Big)^+ - \Big(\frac{\partial}{\partial\tau} u\Big)^-\Big) \cdot v = 0,
\end{aligned}
$$

which proves that the range of $[\nabla_x u]^T$ is contained in the subspace spanned by n.

(ii) Let $m(x,t) = (m'(x,t), m''(x,t)) \in \mathbb{R}^4$ be a unit normal vector to Γ pointing from γ' to γ. With the unit normal vector $n(x,t) = \frac{m'(x,t)}{|m'(x,t)|}$ to $\Gamma(t)$ and with $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^+, \mathbb{R}^3)$ we obtain just as in the proof of Lemma 2.3 that

$$
\begin{aligned}
\Big([C]n\,|\nabla_x S|, \varphi\Big) &= \int_{\Omega\times\mathbb{R}^+} \varphi \cdot [C]n\, d|\nabla_x S| \\
&= \int_\Gamma \varphi(x,t)\cdot[C(x,t)]n(x,t)|m'(x,t)|\, d\sigma_3(x,t) \\
&= \int_\Gamma \Big(\rho[\psi]m' - [(\nabla_x u)^T T]m'\Big)\cdot\varphi\, d\sigma_3 \qquad (2.35) \\
&= \int_\Gamma \rho[\psi]m'\cdot\varphi\, d\sigma_3 - \int_\Gamma \begin{pmatrix} m'\cdot[Tu_{x_1}] \\ \vdots \\ m'\cdot[Tu_{x_3}]\end{pmatrix}\cdot\varphi\, d\sigma_3 \\
&= \int_\Gamma \rho[\psi]m'\cdot\varphi\, d\sigma_3 + \int_{\Omega\times\mathbb{R}^+}\sum_{i=1}^3 \mathrm{div}_x\,(Tu_{x_i}\varphi_i)\, d(x,t)\,.
\end{aligned}
$$

Now, because of the symmetry of T,

$$
\begin{aligned}
&\mathrm{div}_x(Tu_{x_i}\,\varphi_i) = (\mathrm{div}_x T^T)\cdot u_{x_i}\,\varphi_i + T^T : (\nabla_x u_{x_i})\varphi_i + (Tu_{x_i})\cdot\nabla_x\varphi_i \\
&= (\mathrm{div}_x T)\cdot u_{x_i}\,\varphi_i + T : \varepsilon(\nabla_x\, u_{x_i})\varphi_i + (Tu_{x_i})\cdot\nabla_x\,\varphi_i\,. \qquad (2.36)
\end{aligned}
$$

Since S is constant on connected components of $(\Omega\times\mathbb{R}^+)\backslash\Gamma$, we obtain from (2.10) that on $(\Omega\times\mathbb{R}^+)\backslash\Gamma$

$$
\begin{aligned}
T : \varepsilon(\nabla_x\, u_{x_i})\varphi_i &= \rho\nabla_\varepsilon\psi(\varepsilon(\nabla_x u), S, z) : \varepsilon(\nabla_x\, u_{x_i})\varphi_i \\
&= \rho\frac{\partial}{\partial x_i}\,\psi(\varepsilon, S, z)\varphi_i - \rho\nabla_z\psi(\varepsilon, S, z)\cdot z_{x_i}\,\varphi_i\,. \qquad (2.37)
\end{aligned}
$$

Using that T solves (2.1), we obtain by insertion of (2.37) into (2.36) that

$$
\begin{aligned}
&\sum_{i=1}^3 \mathrm{div}_x(Tu_{x_i}\varphi_i) \\
&\quad= \sum_{i=1}^3 \Big(\rho\frac{\partial}{\partial x_i}\,\psi(\varepsilon, S, z) - b\cdot u_{x_i} - \rho\nabla_z\psi(\varepsilon, S, z)\cdot z_{x_i}\Big)\varphi_i \\
&\qquad\qquad + \sum_{i=1}^3 (Tu_{x_i})\cdot\nabla_x\varphi_i \\
&\quad= \Big(\mathrm{div}_x\Big(\rho\psi(\varepsilon, S, z)I\Big) - (\nabla_x u)^T b - \rho(\nabla_x z)^T\nabla_z\psi(\varepsilon, S, z)\Big)\cdot\varphi \\
&\qquad\qquad + (T(\nabla_x u)) : (\nabla_x\varphi)^T\,.
\end{aligned}
$$

We insert this equation into (2.35), note that $(T(\nabla_x u)) : (\nabla_x \varphi)^T = ((\nabla_x u)^T T) : \nabla_x \varphi$ and apply the Divergence Theorem to obtain

$$\begin{aligned}
&\Big([C]n\,|\nabla_x S|, \varphi\Big) \\
&= -\int_{\Omega\times\mathbb{R}^+} \Big(\rho\psi(\varepsilon, S, z)I - (\nabla_x u)^T T\Big) : \nabla_x \varphi \, d(x,t) \\
&\qquad - \int_{\Omega\times\mathbb{R}^+} \Big((\nabla_x u)^T b + \rho(\nabla_x z)^T \nabla_z \psi(\varepsilon, S, z)\Big) \cdot \varphi \, d(x,t) \\
&= \Big(\mathrm{div}_x \Big(\rho\psi(\varepsilon, S, z)I - (\nabla_x u)^T T\Big),\, \varphi\Big) \\
&\qquad - \Big((\nabla_x u)^T b + \rho(\nabla_x z)^T \nabla_z \psi(\varepsilon, S, z),\, \varphi\Big) \\
&= \Big(\mathrm{div}_x C(\nabla_x u, S, z) - (\nabla_x u)^T b - \rho(\nabla_x z)^T \nabla_z \psi(\varepsilon, S, z), \varphi\Big) .
\end{aligned}$$

The second equality sign in this computation holds by definition of the distribution $\mathrm{div}_x\,(\rho\psi I - (\nabla_x u)^T T)$. This proves the lemma.

With this result we obtain the evolution equation for S, which does not contain normal vectors:

Theorem 2.5 *Assume that* $(u, T, z, S) : \Omega \times \mathbb{R}_0^+ \to \mathbb{R}^3 \times \mathcal{S}^3 \times \mathbb{R}^N \times \{0, 1\}$ *satisfies the equations* (2.28)–(2.31)*, the interface conditions*

$$[u] = [T]n = 0$$

on Γ *and the regularity assumptions of Theorem 2.1. Moreover, assume that the function* f *in* (2.30) *fulfills the dissipation inequality* (2.18)*:*

$$\rho\nabla_z\psi(\varepsilon, S, z) \cdot f(S, T, z) \le 0.$$

Then the equation

$$|S_t| = c\,|\mathrm{div}_x\, C(\nabla_x u, S, z) - \rho(\nabla_x z)^T \nabla_z \psi(\varepsilon, S, z) - (\nabla_x u)^T b| \tag{2.38}$$

and the entropy condition

$$\rho\frac{\partial}{\partial t}\,\psi(\varepsilon, S, z) - \mathrm{div}_x\, q(\varepsilon, u_t, S, z) - b \cdot u_t \le 0 \tag{2.39}$$

are satisfied with

$$q(\varepsilon, u_t, S, z) = T u_t\, .$$

Proof: The equations (2.31), (2.32) and (2.33) together imply

$$\begin{aligned}
|S_t| &= c|n \cdot [C]n|\,|\nabla_x S| = c|[C]n|\,|\nabla_x S| \\
&= c\Big|[C]n|\nabla_x S|\Big| = c|\mathrm{div}_x C - \rho(\nabla_x z)^T \nabla_z \psi - (\nabla_x u)^T b|\,,
\end{aligned}$$

which is (2.38). If (2.31) holds, then it follows from Lemma 2.3 that

$$c(n \cdot [C(\nabla_x u, S, z)]n)$$

must be the normal velocity ν of the surface Γ, along which S has a jump. Therefore equation (2.17) is satisfied. By Corollary 2.2, the equations (2.17) and (2.18) together imply that (2.39) holds. This proves the theorem.

Initial-boundary value problem for an inelastic material with evolving microstructure. The equation (2.38) does not contain normal vectors. However, because of the absolute values on both sides, this equation allows more solutions than (2.31) does. We surmise that the entropy condition (2.39) singles out the correct solutions of (2.38) and that, therefore, (2.38) and (2.39) together are equivalent to (2.31). The mathematical model for the inelastic material with evolving microstructure thus derived consists of the equations (2.28)–(2.30), (2.38), of the entropy condition (2.39) as side condition, and of the interface, boundary and initial conditions (2.4)–(2.8). The complete initial-boundary value problem is formulated at the beginning of Section 3.

2.5 Reduction of the evolution equation for smooth solutions

In this section we show that the evolution equation (2.38) can be simplified considerably under the assumption that the function (u, T, z, S) does not jump at the phase boundaries, but varies smoothly in all of $\Omega \times \mathbb{R}^+$. In these investigations we are led by the idea that the initial-boundary value problem consisting of the equations (2.1)–(2.3), (2.7), (2.8) and of the simplified evolution equation derived below has smooth solutions, at least for a finite interval of time, if smooth functions are inserted for the initial data $z^{(0)}$, $S^{(0)}$ in (2.8). We surmise that if a sequence of smooth initial data is chosen, which approximates the original initial data with jumps, a sequence of smooth solutions is obtained approximating the discontinuous solution to the original initial data. This would be helpful both to prove existence of solutions of the initial-boundary value problem (2.1)–(2.8), (2.38) to discontinuous initial data, and to compute the solution of this problem numerically.

Let $J \subseteq \mathbb{R}$ be an interval containing the numbers 0 and 1 and let

$$\begin{aligned}
&\varepsilon^* : J \to \mathcal{S}^3, \\
&f : \Delta(f) \subseteq J \times \mathcal{S}^3 \times \mathbb{R}^N \to \mathbb{R}^N, \\
&\psi : \Delta(\psi) \subseteq \mathcal{S}^3 \times J \times \mathbb{R}^N \to \mathbb{R}
\end{aligned}$$

be smooth functions. We assume that the free energy ψ satisfies (2.10) and that f and ψ satisfy the dissipation inequality (2.18):

$$\rho \nabla_z \psi(\varepsilon, S, z) \cdot f(S, T(\varepsilon, S, z), z) \leq 0$$

for all $(\varepsilon, S, z) \in \Delta(\psi) \cap \{(\varepsilon, S, z) \mid (S, T(\varepsilon, S, z), z) \in \Delta(f)\}$. Here we set

$$T(\varepsilon, S, z) = D(S)(\varepsilon - \varepsilon^*(S) - Bz).$$

Lemma 2.6 *Let (u, T, z, S) be a continuously differentiable solution of the equations (2.28) and (2.38). Then*

$$|S_t| = c\rho |\psi_S(\varepsilon(\nabla_x u), S, z)|\, |\nabla_x S| \tag{2.40}$$

holds in $\Omega \times \mathbb{R}^+$.
Conversely, if (u, T, z, S) is a continuously differentiable solution of

$$\begin{aligned} -\mathrm{div}_x T &= b, & (2.41)\\ T &= D(S)\Big(\varepsilon(\nabla_x u) - \varepsilon^*(S) - Bz\Big), & (2.42)\\ z_t &= f(S, T, z), & (2.43)\\ S_t &= -c\rho\, \psi_S(\varepsilon(\nabla_x u), S, z)\, |\nabla_x S|, & (2.44) \end{aligned}$$

then (2.28)–(2.30), the evolution equation (2.38) for S and the entropy condition (2.39) are satisfied.

Proof: The definition of the Eshelby tensor in (2.15) yields

$$\begin{aligned} &\mathrm{div}_x C - \rho(\nabla_x z)^T \nabla_z \psi - (\nabla_x u)^T b & (2.45)\\ &= \rho \nabla_x \psi - \mathrm{div}_x\Big((\nabla_x u)^T T\Big) - \rho(\nabla_x z)^T \nabla_z \psi - (\nabla_x u)^T b\,. \end{aligned}$$

Moreover, (2.10) implies

$$\begin{aligned} &\rho \nabla_x \psi(\varepsilon, S, z)\\ &= \begin{pmatrix} \rho \nabla_\varepsilon \psi(\varepsilon, S, z) : \varepsilon_{x_1} + \rho \nabla_z \psi(\varepsilon, S, z) \cdot z_{x_1} \\ \vdots \\ \rho \nabla_\varepsilon \psi(\varepsilon, S, z) : \varepsilon_{x_3} + \rho \nabla_z \psi(\varepsilon, S, z) \cdot z_{x_3} \end{pmatrix} + \rho \psi_S(\varepsilon, S, z) \nabla_x S\\ &= \begin{pmatrix} T : \varepsilon_{x_1} \\ \vdots \\ T : \varepsilon_{x_3} \end{pmatrix} + \rho (\nabla_x z)^T \nabla_z \psi + \rho \psi_S(\varepsilon, S, z) \nabla_x S\,. \end{aligned} \tag{2.46}$$

Also, because of the symmetry of T,

$$\begin{aligned} -\mathrm{div}_x\Big((\nabla_x u)^T T\Big) &= -(\nabla_x u)^T \mathrm{div}_x T - \begin{pmatrix} T : \nabla_x(u_{x_1}) \\ \vdots \\ T : \nabla_x(u_{x_3}) \end{pmatrix}\\ &= -(\nabla_x u)^T \mathrm{div}_x T - \begin{pmatrix} T : \varepsilon_{x_1} \\ \vdots \\ T : \varepsilon_{x_3} \end{pmatrix}. \end{aligned} \tag{2.47}$$

Therefore, if T solves (2.28) (or (2.41)), then we obtain by combination of (2.45)–(2.47) the equality

$$\operatorname{div}_x C - \rho(\nabla_x z)^T \nabla_z \psi - (\nabla_x u)^T b = \rho \psi_S(\varepsilon, S, z)\, \nabla_x S\,. \tag{2.48}$$

With this equation the proof of the lemma readily follows: First, if (2.28) and (2.38) are satisfied, then insertion of (2.48) in (2.38) yields (2.40). Conversely, if (2.41)–(2.44) are satisfied, we take absolut values on both sides of (2.44) and insert (2.48) into the resulting equation to obtain (2.38). The equations (2.28)–(2.30) hold, since (2.41)–(2.43) are restatements of these equations.

To prove that the entropy condition (2.39) holds, we use (2.20) and (2.41) to compute

$$\begin{aligned}
&\rho \frac{\partial}{\partial t} \psi(\varepsilon, S, z) - \operatorname{div}_x q(\varepsilon, u_t, S, z) - b \cdot u_t \\
&= \rho(\nabla_\varepsilon \psi) : \varepsilon(\nabla_x u_t) + \rho \psi_S\, S_t + \rho \nabla_z \psi \cdot z_t \\
&\qquad\qquad - (\operatorname{div}_x T) \cdot u_t - \rho(\nabla_\varepsilon \psi) : \varepsilon(\nabla_x u_t) - b \cdot u_t \\
&= \rho \psi_S S_t + \rho \nabla_z \psi \cdot z_t \\
&= -\rho \psi_S\, c \rho \psi_S |\nabla_x S| + \rho \nabla_z \psi \cdot f \le 0.
\end{aligned}$$

The last equality sign follows from (2.43) and (2.44), and the inequality sign is a consequence of the dissipation inequality (2.18) for f, which we assumed to hold. This shows that the entropy condition (2.39) is fulfilled.

Scholia. *1.* Because of the product $\psi_S\,|\nabla_x S|$, the formulation of the system (2.41)–(2.44) is only valid for smooth solutions. Since a smooth solution of this system also satisfies the evolution equation (2.38) and the entropy condition (2.39), whose formulations are both valid for non-smooth solutions, it is tempting to assume that for a sequence of smooth solutions tending to a non-smooth limit function, this limit function is a solution of (2.38) and (2.39). This would allow us to construct and compute numerically non-smooth solutions of the initial-boundary value problem for evolving microstructures using the simpler equations (2.41)–(2.44).

2. In this section we require that the free energy $\psi(\varepsilon, S, z)$ is defined for all values of S in an interval J containing 0 and 1. As in the derivation of the Cahn-Allen equation, cf. [9], it should be required that ψ is a double well potential having minima at the values $S = 0$ and $S = 1$. The first order equations (2.44) or (2.38) could be an alternative to the Cahn-Allen equation, an equation of second order.

3 Homogenization of the equations for materials with evolving microstructure

3.1 The microscopic initial-boundary value problem

In this section we study the homogenization of the following initial-boundary value problem for (u, T, z, S) stated and derived in the preceding section: In $\Omega \times \mathbb{R}^+$ the partial differential equations

$$
\begin{aligned}
-\mathrm{div}_x\, T(x,t) &= b(x,t) && (3.1)\\
T(x,t) &= D(S(x,t))\Big(\varepsilon(\nabla_x\, u(x,t)) - \varepsilon^*(S(x,t)) - Bz(x,t)\Big) && (3.2)\\
z_t(x,t) &= f(S(x,t),\, T(x,t),\, z(x,t)) && (3.3)\\
|S_t(x,t)| &= \eta c|\mathrm{div}_x\, C(\nabla_x u, S, z) \\
&\quad -\rho(\nabla_x\, z)^T \nabla_z\, \psi(\varepsilon(\nabla_x\, u), S, z) - (\nabla_x\, u)^T b| && (3.4)
\end{aligned}
$$

must be satisfied. The entropy condition

$$
\rho \frac{\partial}{\partial t}\psi(\varepsilon, S, z) - \mathrm{div}_x\,(T u_t) - b u_t \le 0\,, \tag{3.5}
$$

must be fulfilled as side condition. The interface conditions are

$$
[u(x,t)] = [T(x,t)]n(x,t) = 0, \quad z(x,t+) = g(z(x,t-)), \quad (x,t) \in \Gamma, \tag{3.6}
$$

the boundary condition is

$$
T(x,t)n(x) = 0, \quad x \in \partial\Omega,\ t \ge 0\,, \tag{3.7}
$$

and the initial conditions are

$$
z(x,0) = z^{(0)}(x)\,, \quad S(x,0) = S^{(0)}(x), \quad x \in \Omega\,. \tag{3.8}
$$

In the interface condition $g : \mathbb{R}^N \to \mathbb{R}^N$ is a given function.

At time $t = 0$ the microstructure in the material, that is the distribution of the γ'–precipitates in the γ–matrix phase, is determined by the initial function $S^{(0)}$. We shall assume that the microstructure is approximately periodic at $t = 0$ and study the situation when the dimensions of the periodicity cell of this microstructure are proportional to a parameter η and thus tend to zero for $\eta \to 0$. If we assume that also the initial function $z^{(0)}$ is approximately periodic with the same periodicity cell, then also the solution (u, T, z, S) of (3.1)–(3.8) to these initial data will be periodic. With shrinking periodicity cell one expects that this solution tends in a suitable sense against the solution of a homogenized system of partial differential equations. In this section we derive this homogenized system.

This derivation will be purely formal, however, since we do neither prove that the initial-boundary value problem (3.1)–(3.8) has a solution, nor do we prove that solutions must converge to solutions of the homogenized system. Instead, we assume that solutions of this initial-boundary value problem exist and that these solutions converge to limit functions. Our goal is to derive a system of partial differential equations, the homogenized system, which must be satisfied by the limit functions.

The constant ηc in (3.4) determines the speed of propagation of the phase boundary between the γ– and γ'–phases. Since this speed is proportional to η, it is also proportional to the dimensions and distances of the precipitates. The time scale, on which the microstructure evolves, does therefore not change if η tends to zero. If the speed of propagation would not decrease with η, then because of the decreasing distances of the precipitates the microstructure would evolve more and more rapidly, and the interaction of the precipitates would happen in a short time interval with length tending to zero. One expects that after this short time interval the microstructure would settle to an approximately steady state. Homogenization would essentially amount to determine an initial-boundary value problem, whose solutions are asymptotic to the solution of the original problem at large times.

At present we do not know how to derive such an initial-boundary value problem. In fact, in practical problems the main interest is not to determine such a long time asymptotics to the evolution of the microstructure. Instead, in a real material the evolution of the microstructure is slow and typically needs hundreds or thousands of hours, and it is just this slow evolution before and during the interaction and the formation of the plate-like structure, which one wants to study. The choice of the constant ηc in (3.4) is therefore not only justified by the reduction of the mathematical difficulties; it is in fact a natural choice in the problem we want to study.

The evolution equation (3.4) for the order parameter and the equation resulting from it in the homogenized initial-boundary value problem are distribution equations. To derive and formulate the homogenized distribution equation we use *a family of solutions of the initial-boundary value problem* (3.1)–(3.8) *depending on the fast variable.* The definition of this family is given below. The homogenized equations for the displacement, the stress and the internal variables are derived in Section 3.2 using the method of asymptotic series. In Section 3.3 we prove some results for oscillating functions of bounded variation, which are used in Section 3.4 to derive the homogenized equation for the order parameter. There we also formulate the complete homogenized initial-boundary value problem.

Thus, assume that the initial data are given in the form

$$z^{(0)}(x) = z_0^{(0)}(x, \frac{x}{\eta}), \quad S^{(0)}(x) = S_0^{(0)}(x, \frac{x}{\eta}), \tag{3.9}$$

with a parameter $\eta > 0$ and functions $z_0^{(0)} : \Omega \times \mathbb{R}^3 \to \mathbb{R}^N$, $S_0^{(0)} : \Omega \times \mathbb{R}^3 \to \{0, 1\}$. The functions $y \mapsto z_0^{(0)}(x, y)$, $y \mapsto S_0^{(0)}(x, y)$ are assumed to be periodic for every $x \in \Omega$ with a bounded periodicity cell $Y \subseteq \mathbb{R}^3$. For simplicity we assume that

$$\int_Y dy = 1. \tag{3.10}$$

We consider values of η in the range $0 < \eta < \eta_0$ with a positive constant η_0. The functions $z_0^{(0)}(x, \frac{x}{\eta})$ and $S_0^{(0)}(x, \frac{x}{\eta})$ are approximately periodic with a periodicity cell, whose dimensions decrease to zero when η tends to zero.

In the following definition the value $\eta > 0$ is kept fixed:

Definition 3.1 *Let*

$$((x, y, t) \mapsto (u, T, z, S)) : \Omega \times \mathbb{R}^3 \times \mathbb{R}^+ \to \mathbb{R}^3 \times \mathcal{S}^3 \times \mathbb{R}^N \times \{0, 1\}$$

be a function which satisfies the initial condition

$$z(x, y, 0) = z_0^{(0)}(x, \frac{x}{\eta} + y), \quad S(x, y, 0) = S_0^{(0)}(x, \frac{x}{\eta} + y) \tag{3.11}$$

for almost all $(x, y) \in \Omega \times \mathbb{R}^3$*, and for which the function* $(x, t) \mapsto (u, T, z, S)(x, y, t)$ *is a solution of* (3.1)–(3.7) *for almost all* $y \in \mathbb{R}^3$*. Then* (u, T, z, S) *is called a family of solutions depending on the fast variable* y *of the initial-boundary value problem* (3.1)–(3.7), (3.11) *with parameter* η *and initial data* $(z_0^{(0)}, S_0^{(0)})$*.*

In the following we fix $z_0^{(0)}$ and $S_0^{(0)}$ and for brevity avoid to mention the initial data. Thus, we call (u, T, z, S) a family of solutions of the initial-boundary value problem depending on the fast variable with parameter η.

3.2 Homogenized equations for u, T and z

In this section we study the homogenization of the equations (3.1)–(3.3). We assume that for all $0 < \eta < \eta_0$ a family of solutions $(\hat{u}_\eta, \hat{T}_\eta, \hat{z}_\eta, \hat{S}_\eta)$ of the initial-boundary value problem depending on the fast variable with parameter η exists, which can be asymptotically expanded in the form

$$(\hat{u}_\eta, \hat{T}_\eta, \hat{z}_\eta, \hat{S}_\eta)(x, y, t) = (u_\eta, T_\eta, z_\eta, S_\eta)(x, \frac{x}{\eta} + y, t), \quad 0 < \eta < \eta_0, \tag{3.12}$$

with

$$u_\eta(x,y,t) \;=\; u_0(x,t) + \eta u_1(x,y,t) + \eta^2 u_2(x,y,t,\eta) \tag{3.13}$$

$$T_\eta(x,y,t) \;=\; T_0(x,y,t) + \eta T_1(x,y,t,\eta) \tag{3.14}$$

$$z_\eta(x,y,t) \;=\; z_0(x,y,t) + z_1(x,y,t,\eta) \tag{3.15}$$

$$S_\eta(x,y,t) \;=\; S_0(x,y,t) + S_1(x,y,t,\eta)\,, \tag{3.16}$$

where the functions

$$u_\eta,\ u_1,\ u_2(\cdot,\eta) : \Omega \times \mathbb{R}^3 \times \mathbb{R}^+ \to \mathbb{R}^3$$

$$T_\eta,\ T_0,\ T_1(\cdot,\eta) : \Omega \times \mathbb{R}^3 \times \mathbb{R}^+ \to \mathcal{S}^3$$

$$z_\eta,\ z_0,\ z_1(\cdot,\eta) : \Omega \times \mathbb{R}^3 \times \mathbb{R}^+ \to \mathbb{R}^N$$

$$S_\eta,\ S_0,\ S_1(\cdot,\eta) : \Omega \times \mathbb{R}^3 \times \mathbb{R}^+ \to \{0,\,1\}$$

are assumed to be periodic with respect to the y–argument and have periodicity cell Y. The remainder terms are assumed to satisfy

$$\lim_{\eta\to 0} S_1(x,y,t,\eta) \;=\; 0 \tag{3.17}$$

$$\lim_{\eta\to 0} \int_\Omega \int_Y |z_1(x,y,t,\eta)|^2 dydx \;=\; 0\,, \tag{3.18}$$

and the boundedness conditions

$$\sup_{0<\eta<\eta_0} \int_\Omega \int_Y \left(|D^\alpha_{x,y}\, u_2(x,y,t,\eta)|^2 \right) dydx < \infty \tag{3.19}$$

$$\sup_{0<\eta<\eta_0} \int_\Omega \int_Y \left(|D^\alpha_{x,y}\, T_1(x,y,t,\eta)|^2 \right) dydx < \infty, \tag{3.20}$$

for every multi-index α with $|\alpha| \le 1$.

Scholia. *1.* The function $(\hat z_\eta, \hat S_\eta)$ satisfies the initial condition (3.11) if (z_η, S_η) fulfills

$$z_\eta(x,y,0) = z_0^{(0)}(x,y), \quad S_\eta(x,y,0) = S_0^{(0)}(x,y), \quad (x,y) \in \Omega \times \mathbb{R}^3.$$

2. If the solution of the initial-boundary value problem (3.1)–(3.8) is unique, and if $(\hat u_\eta, \hat T_\eta, \hat z_\eta, \hat S_\eta)$ is a family of solutions to the initial-boundary value problem (3.1)–(3.7), (3.11) depending on the fast variable with parameter η, then $y \mapsto (\hat u_\eta, \hat T_\eta, \hat z_\eta, \hat S_\eta)(x,y,t)$ is periodic with periodicity cell Y. For, otherwise a solution different from

$$(\hat u_\eta, \hat T_\eta, \hat z_\eta, \hat S_\eta) : \Omega \times \mathbb{R}^3 \times \mathbb{R}^+_0 \to \mathbb{R}^3 \times \mathcal{S}^3 \times \mathbb{R}^N \times \{0,\,1\}$$

could be obtained by extending $(\hat{u}_\eta, \hat{T}_\eta, \hat{z}_\eta, \hat{S}_\eta)|_{\Omega\times Y\times\mathbb{R}_0^+}$ periodically with periodicity cell $\Omega \times Y \times \mathbb{R}_0^+$ to $\Omega \times \mathbb{R}^3 \times \mathbb{R}_0^+$. This would contradict the uniqueness of the solution.

3. Assume that $(\hat{u}_\eta, \hat{T}_\eta, \hat{z}_\eta, \hat{S}_\eta)$ is a family of solutions depending on the fast variable with parameter η, which are periodic with respect to the y–argument and have periodicity cell Y. Let $(u_0, u_1, T_0, z_0, S_0) = (u_0, u_1, T_0, z_0, S_0)(x, y, t)$ be a given function, which is periodic with respect to y and has periodicity cell Y. Then necessarily the remainder $(\tilde{u}, \tilde{T}, \tilde{z}, \tilde{S})$ defined by

$$\begin{aligned}&(\hat{u}_\eta, \hat{T}_\eta, \hat{z}_\eta, \hat{S}_\eta)(x, y, t) \\ &= (u_0 + \eta u_1, T_0, z_0, S_0)(x, \frac{x}{\eta} + y, t) + (\eta^2 \tilde{u}, \eta\tilde{T}, \tilde{z}, \tilde{S})(x, y, t, \eta)\end{aligned} \tag{3.21}$$

is of the form given above:

$$(\tilde{u}, \tilde{T}, \tilde{z}, \tilde{S})(x, y, t, \eta) = (u_2, T_1, z_1, S_1)(x, \frac{x}{\eta} + y, t, \eta)\,, \tag{3.22}$$

with a function

$$(x, y, t) \mapsto (u_2, T_1, z_1, S_1)(x, y, t, \eta),$$

which is periodic with respect to y and has periodicity cell Y. For, the left hand side of the equation (3.21) and the first term on the right hand side are periodic with periodicity cell Y. Therefore also the second term on the right hand side is periodic. Define

$$(u_2, T_1, z_1, S_1)(x, y, t, \eta) = (\tilde{u}, \tilde{T}, \tilde{z}, \tilde{S})(x, y - \frac{x}{\eta}, t, \eta).$$

Clearly, $u_2,\ T_1,\ z_1,\ S_1$ are periodic with respect to y and satisfy (3.22).

Homogenization. From the hypothesis that $(\hat{u}_\eta, \hat{T}_\eta, \hat{z}_\eta, \hat{S}_\eta)$ is a family of solutions of the initial-boundary value problem depending on the fast variable and under the assumption that the terms u_2 and T_1 in the asymptotic expansion satisfy (3.19) and (3.20) we derive now a system of three equations which must be satisfied by the limit functions $u_0,\ T_0,\ z_0,\ S_0$. The equations of this system are the homogenized equations corresponding to the equations (3.1)–(3.3). To formulate this system we need some definitions:

By $M_Y : L^2(Y) \to \mathbb{R}$ we denote the mean value operator

$$M_Y v = \int_Y v(y)\, dy\,.$$

Of course, M_Y can also be considered to be a projector to the space of constant functions on Y.

The elasticity tensors $D(0) : \mathcal{S}^3 \to \mathcal{S}^3$ and $D(1) : \mathcal{S}^3 \to \mathcal{S}^3$ in the matrix phase γ and in the γ'–phase, respectively, are by assumption symmetric, positive definite mappings. Since the inverses $D(0)^{-1}$ and $D(1)^{-1}$ have the same properties, to a given function $S : \Omega \times Y \times \mathbb{R}_0^+ \to \{0, 1\}$ we can therefore define an (S, x, t)–dependent scalar product on $L^2(Y, \mathcal{S}^3)$ by

$$[v, w]_{(S,x,t)} = \int_Y \Big(D(S(x, y, t))^{-1} v(y) \Big) : w(y)\, dy \,,$$

for $v,\, w \in L^2(Y, \mathcal{S}^3)$. Let

$$\begin{aligned} \mathcal{D}_0 \quad = \quad \Big\{ w\big|_Y \;\Big|\; & w \in L^{2,\mathrm{loc}}(\mathbb{R}^3, \mathcal{S}^3),\ \operatorname{div}_y w = 0,\ w \text{ is periodic} \\ & \qquad\qquad\qquad\qquad \text{with periodicity cell } Y \Big\} \,. \end{aligned}$$

$\mathcal{D}_0$ is a closed subspace of $L^2(Y, \mathcal{S}^3)$. By

$$P_{(S,x,t)} : L^2(Y, \mathcal{S}^3) \to \mathcal{D}_0 \subseteq L^2(Y, \mathcal{S}^3)$$

we denote the projector onto $\mathcal{D}_0$, which is orthogonal with respect to the scalar product $[v, w]_{(S,x,t)}$. Of course, $P_{(S,x,t)}$ depends on the function S and on (x, t).

By $H_1(\Omega \times Y)$ we denote the usual Sobolev space of functions with weak derivatives in $L^2(\Omega \times Y)$ up to order 1.

Theorem 3.2 *Assume that for all $\eta_0 > \eta > 0$ the function $(\hat{u}_\eta, \hat{T}_\eta, \hat{z}_\eta, \hat{S}_\eta)$ with the representation* (3.12)–(3.16) *is a family of solutions of the initial-boundary value problem depending on the fast variable with parameter η. If the function $(x, y) \mapsto (u_0, u_1, u_2, T_0, T_1)(x, y, t)$ belongs to the Sobolev space $H_1(\Omega \times Y)$ for almost all t, if $(x, y) \mapsto (z_0, z_1)(x, y, t)$ belongs to $L^2(\Omega \times Y)$ for almost all t, and if the conditions* (3.17)–(3.20) *are fulfilled, then the function (u_0, T_0, z_0, S_0) satisfies*

$$-\operatorname{div}_x \left(M_Y T_0(x, \cdot, t) \right) \;=\; b(x, t) \tag{3.23}$$

$$\begin{aligned} T_0(x, \cdot, t) \;=\; & P_{(S_0,x,t)} \Big\{ D(S_0(x, \cdot, t)) \Big(\varepsilon(\nabla_x u_0(x, t)) \\ & - \varepsilon^*(S_0(x, \cdot, t)) - B z_0(x, \cdot, t) \Big) \Big\} \,. \end{aligned} \tag{3.24}$$

Proof: From (3.12) and (3.14) we obtain

$$\begin{aligned} &\operatorname{div}_x \hat{T}_\eta(x, y, t) = \operatorname{div}_x T_\eta(x, \frac{x}{\eta} + y, t) \\ &= \operatorname{div}_x \Big(T_0(x, \frac{x}{\eta} + y, t) + \eta T_1(x, \frac{x}{\eta} + y, t, \eta) \Big) \end{aligned}$$

$$= \Big[\frac{1}{\eta}\mathrm{div}_\xi\, T_0(x,\xi,t) \tag{3.25}$$
$$+ \mathrm{div}_x\, T_0(x,\xi,t) + \mathrm{div}_\xi\, T_1(x,\xi,t,\eta)$$
$$+ \eta \mathrm{div}_x\, T_1(x,\xi,t,\eta)\Big]_{\xi=\frac{x}{\eta}+y}.$$

Because of the periodicity of $y \mapsto T_1(x,y,t,\eta)$, the hypothesis (3.20) implies

$$\eta\Big(\int_\Omega\int_Y |\mathrm{div}_x\, T_1(x,\xi,t,\eta)|_{\xi=\frac{x}{\eta}+y}|^2 dydx\Big)^{1/2}$$
$$= \eta\Big(\int_\Omega\int_Y |\mathrm{div}_x T_1(x,y,t,\eta)|^2 dydx\Big)^{1/2} \le \eta K_1\,,$$

with a suitable constant K_1. This estimate and (3.25) show that (3.1) can only hold for all $0 < \eta < \eta_0$ if

$$\int_\Omega\int_Y |\mathrm{div}_y\, T_0(x,\frac{x}{\eta}+y,t)|^2 dydx = \int_\Omega\int_Y |\mathrm{div}_y\, T_0(x,y,t)|^2 dydx = 0$$

and

$$\int_\Omega\int_Y |\mathrm{div}_x T_0(x,\xi,t)|_{\frac{x}{\eta}+y} + \mathrm{div}_y\, T_1(x,\frac{x}{\eta}+y,t,\eta) + b(x,t)|^2 dydx$$
$$= \int_\Omega\int_Y |\mathrm{div}_x T_0(x,y,t) + \mathrm{div}_y\, T_1(x,y,t,\eta) + b(x,t)|^2 dydx = 0,$$

from which we conclude that the equations

$$\mathrm{div}_y\, T_0(x,y,t) = 0 \tag{3.26}$$
$$-\mathrm{div}_x\, T_0(x,y,t) - \mathrm{div}_y\, T_1(x,y,t,\eta) = b(x,t) \tag{3.27}$$

hold for almost all $(x,y,t) \in \Omega \times \mathbb{R}^3 \times \mathbb{R}^+$. Integration of (3.27) with respect to y yields

$$-\mathrm{div}_x \int_Y T_0(x,y,t)\, dy - \int_Y \mathrm{div}_y\, T_1(x,y,t,\eta)\, dy = \int_Y b(x,t)\, dy = b(x,t)\,,$$

where in the last step we used (3.10). The Divergence Theorem yields

$$-\mathrm{div}_x \int_Y T_0(x,y,t)\, dy - \int_{\partial Y} T_1(x,y,t,\eta) n(y)\, d\sigma(y) = b(x,t)\,, \tag{3.28}$$

where $n(y)$ is the exterior unit normal vector to ∂Y at y. Since Y is a periodicity cell for T_1, it follows that

$$\int_{\partial Y} T_1(x,y,t,\eta) n(y)\, d\sigma(y) = 0\,.$$

With the definition of the mean value operator equation (3.28) can therefore be written in the form of equation (3.23).

To prove (3.24), we insert (3.13) and (3.14) into (3.2) and obtain for $\xi = \frac{x}{\eta} + y$

$$\begin{aligned}
&T_0(x,\xi,t) + \eta T_1(x,\xi,t,\eta) \\
&= D(S_\eta(x,\xi,t))\Big(\varepsilon(\nabla_x u_0(x,t) + \nabla_\xi u_1(x,\xi,t)) \\
&\qquad + \eta\varepsilon(\nabla_x u_1(x,\xi,t) + \nabla_\xi u_2(x,\xi,t,\eta)) \\
&\qquad + \eta^2\varepsilon(\nabla_x u_2(x,\xi,t,\eta)) - \varepsilon^*(S_\eta(x,\xi,t)) - Bz_\eta(x,\xi,t)\Big)\,.
\end{aligned} \tag{3.29}$$

With the components $D_{ijkl}(S)$ of the elasticity tensor $D(S)$ we define

$$|D(S)|^2 = \sum D_{ijkl}(S)^2.$$

Since the hypothesis (3.17) implies

$$\lim_{\eta\to 0} |D(S_\eta(x,y,t)) - D(S_0(x,y,t))|^2 = 0$$

for almost all (x,y), since S_η and S_0 have values in $\{0,\, 1\}$ and since all functions are periodic with respect to y, the Dominated Convergence Theorem implies

$$\begin{aligned}
&\lim_{\eta\to 0} \int_\Omega \int_Y \Big| \Big(D(S_\eta(x, \frac{x}{\eta} + y, t)) - D(S_0(x, \frac{x}{\eta} + y, t)) \Big) \\
&\qquad\qquad \Big(\varepsilon(\nabla_x u_0(x,t) + \nabla_y u_1(x, \frac{x}{\eta} + y, t)) \Big) \Big|\, dydx \\
&= \lim_{\eta\to 0} \int_\Omega \int_Y \Big| \Big(D(S_\eta(x,y,t)) - D(S_0(x,y,t)) \Big) \\
&\qquad\qquad \Big(\varepsilon(\nabla_x u_0(x,t) + \nabla_y u_1(x,y,t)) \Big) \Big|\, dydx \\
&\le \lim_{\eta\to 0} \Big(\int_\Omega \int_Y \Big| D(S_\eta(x,y,t)) - D(S_0(x,y,t)) \Big|^2 dydx \Big)^{1/2} \\
&\qquad \cdot \Big(\int_\Omega \int_Y \Big| \varepsilon(\nabla_x u_0(x,t) + \nabla_y u_1(x,y,t)) \Big|^2 dydx \Big)^{1/2} = 0\,.
\end{aligned} \tag{3.30}$$

Since $|D(S_\eta(x,y,t))| \le \max(|D(0)|, |D(1)|)$, the hypothesis (3.19) yields

$$\lim_{\eta\to 0}\int_\Omega\int_Y \Big|D(S_\eta(x,\frac{x}{\eta}+y,t))\Big(\eta\varepsilon(\nabla_x u_1(x,\xi,t) + \nabla_\xi u_2(x,\xi,t,\eta)) + \eta^2\varepsilon(\nabla_x u_2(x,\xi,t,\eta))\Big)_{|\frac{x}{\eta}+y}\Big|\, dydx$$
$$\le \lim_{\eta\to 0}\Big(\int_\Omega\int_Y |D(S_\eta(x,y,t))|^2 dydx\Big)^{1/2} \Big(\int_\Omega\int_Y |\eta\varepsilon(\nabla_x u_1 + \nabla_y u_2) + \eta^2\varepsilon(\nabla_x u_2)|^2 dydx\Big)^{1/2} = 0 \tag{3.31}$$

By a similar reasoning we see that (3.15)–(3.18) and the Dominated Convergence Theorem also imply

$$\lim_{\eta\to 0}\int_\Omega\int_Y \Big|D(S_\eta(x,\frac{x}{\eta}+y,t))\Big(\varepsilon^*(S_\eta(x,\frac{x}{\eta}+y,t)) - Bz_\eta(x,\frac{x}{\eta}+y,t)\Big)$$
$$-D(S_0(x,\frac{x}{\eta}+y,t))\Big(\varepsilon^*(S_0(x,\frac{x}{\eta}+y,t)) - Bz_0(x,\frac{x}{\eta}+y,t)\Big)\Big| dydx = 0. \tag{3.32}$$

Finally, (3.20) implies

$$\lim_{\eta\to 0}\int_\Omega\int_Y |\eta T_1(x,\frac{x}{\eta}+y,t,\eta)|\, dx \le |\Omega|^{1/2}\lim_{\eta\to 0}\eta\Big(\int_\Omega\int_Y |T_1(x,y,t,\eta)|^2 dydx\Big)^{1/2} = 0\,. \tag{3.33}$$

Combination of (3.30)–(3.33) with (3.29) shows that (3.2) can hold for all $\eta_0 > \eta > 0$ only if

$$\int_\Omega\int_Y \Big|T_0(x,\xi,t) - D(S_0(x,\xi,t))\Big(\varepsilon(\nabla_x u_0(x,t) + \nabla_\xi u_1(x,\xi,t)) - \varepsilon^*(S_0(x,\xi,t)) - Bz_0(x,\xi,t)\Big)\Big|_{\xi=\frac{x}{\eta}+y} dydx$$
$$= \int_\Omega\int_Y \Big|T_0(x,y,t) - D(S_0(x,y,t))\Big(\varepsilon(\nabla_x u_0(x,t) + \nabla_y u_1(x,y,t)) - \varepsilon^*(S_0(x,y,t)) - Bz_0(x,y,t)\Big)\Big|\, dydx = 0,$$

where we again used the periodicity of all functions of the integrand with respect to y, whence

$$
\begin{aligned}
T_0(x,y,t) \;\; &= \;\; D(S_0(x,y,t))\Big(\varepsilon(\nabla_x u_0(x,t)+\nabla_y u_1(x,y,t)) \\
&\qquad\qquad - \varepsilon^*(S_0(x,y,t)) - Bz_0(x,y,t)\Big)
\end{aligned} \tag{3.34}
$$

for almost all $(x,y,t)\in\Omega\times\mathbb{R}^3\times\mathbb{R}^+$.

To see that this equation implies (3.24), note that for every $w\in\mathcal{D}_0$ we obtain because of the symmetry of $w(y)$ for the scalar product

$$
\begin{aligned}
&[D(S_0(x,\cdot,t))\,\varepsilon(\nabla_y u_1(x,\cdot,t)),\, w(\cdot)]_{(S_0,x,t)} \\
&= \int_Y \varepsilon(\nabla_y u_1(x,y,t)) : w(y)\, dy = \int_Y \nabla_y u_1(x,y,t) : w(y)\, dy \\
&= \int_Y u_1(x,y,t)\cdot \operatorname{div} w(y)\, dy = 0\,.
\end{aligned}
$$

The last integral vanishes since $\operatorname{div} w = 0$. The partial integration does not yield boundary terms, since u_1 and w both have periodicity cell Y. From this computation we conclude that the function $y\mapsto D(S_0(x,y,t))\,\varepsilon(\nabla_y u_1(x,y,t))$ belongs to the orthogonal space of $\mathcal{D}_0$. This orthogonal space is equal to the kernel of the projector $P_{(S_0,x,t)}$. Moreover, (3.26) implies that $y\mapsto T_0(x,y,t)$ belongs to $\mathcal{D}_0$. Application of $P_{(S_0,x,t)}$ on both sides of (3.34) thus yields the equation (3.24). This completes the proof.

Remark. For use in Section 3.4 we note that the reasoning at the end of this proof also shows that application of $P^{\perp}_{(S_0,x,t)} = (I - P_{(S_0,x,t)})$ to (3.34) yields

$$
\begin{aligned}
&-D(S_0(x,\cdot,t))\varepsilon(\nabla_y u_1(x,\cdot,t)) \\
&= P^{\perp}_{(S_0,x,t)}\Big\{D(S_0(x,\cdot,t))(\varepsilon(\nabla_x u_0(x,t)) - \varepsilon^*(S_0(x,\cdot,t)) - Bz_0(x,\cdot,t))\Big\}.
\end{aligned} \tag{3.35}
$$

Definition 3.3 *We call the equations*

$$
-\operatorname{div}_x(M_Y T_0(x,\cdot,t)) \;\; = \;\; b(x,t) \tag{3.36}
$$

$$
\begin{aligned}
T_0(x,\cdot,t) \;\; &= \;\; P_{(S_0,x,t)}\{D(S_0(x,\cdot,t))(\varepsilon(\nabla_x u_0(x,t)) \\
&\qquad - \varepsilon^*(S_0(x,\cdot,t)) - Bz_0(x,\cdot,t))\}
\end{aligned} \tag{3.37}
$$

$$
\frac{\partial}{\partial t} z_0(x,y,t) \;\; = \;\; f(S_0(x,y,t), T_0(x,y,t), z_0(x,y,t)) \tag{3.38}
$$

homogenized system associated to the equations (3.1)–(3.3).

Note that we did not require f to satisfy any restricting conditions. In constitutive models used in the engineering sciences f is in general a function growing rapidly with respect to several of its variables. Of course, for such general f the conditions (3.17)–(3.20) for the solution (u,T,z,S) of (3.1)–(3.3) are not sufficient to guarantee that the limit function (T_0,z_0,S_0) satisfies the equation (3.38). Clearly, for a given function f it is not difficult to formulate conditions for (u,T,S,z) assuring that the limit function satisfies (3.38). However, such investigations are of interest only in connection with investigations of existence and regularity of solutions of the initial-boundary value problem (3.1)–(3.8). The justification of (3.38) in the homogenized system is therefore left to later works.

3.3 Oscillating functions of bounded variation

It remains to derive the homogenized form of the evolution equation for the order parameter. The derivatives in this evolution equation are measures. In this section we study the measures obtained by insertion of oscillating solutions of the form (3.12) into this equation. The derivation of the homogenized evolution equation in the next section is based upon the result obtained in the following lemma. To state this lemma, we need some definitions and notations.

Assume that

$$((x,y,t)\mapsto H_\eta(x,y,t))\in BV^{\mathrm{loc}}(\Omega\times\mathbb{R}^3\times\mathbb{R}^+)$$

for all $0<\eta<\eta_0$. The values of H_η can lie in $\mathbb{R}$, in $\mathbb{R}^N$ or in the set $\mathcal{M}^3$ of 3×3–matrices. Accordingly, in this section the scalar product in all three spaces is uniformly denoted by $v\cdot w$, and the test functions are chosen with values in appropriate spaces. We set

$$\hat{H}_\eta(x,y,t)=H_\eta(x,\frac{x}{\eta}+y,t)$$

for $\eta>0$. The distribution $\mathrm{div}_x\hat{H}_\eta$ is defined by

$$(\mathrm{div}_x\hat{H}_\eta,\varphi)=-\int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+}H_\eta(x,\frac{x}{\eta}+y,t)\cdot\nabla_x\varphi(x,y,t)\,d(x,y,t),$$

for $\varphi\in C_0^\infty(\Omega\times\mathbb{R}^3\times\mathbb{R}^+)$. This distribution is a measure. To see this, note that if V is an open set compactly contained in $\Omega\times\mathbb{R}^3\times\mathbb{R}^+$, then also

$$V_\eta=\{(x,y,t)\mid(x,y-\frac{x}{\eta},t)\in V\}$$

is open and compactly contained in $\Omega\times\mathbb{R}^3\times\mathbb{R}^+$. Since $H_\eta\in BV^{\mathrm{loc}}(\Omega\times\mathbb{R}^3\times\mathbb{R}^+)$, the derivatives div_xH_η and div_yH_η are measures. This means that there exist constants $C_1,\ C_2$ with

$$|(\mathrm{div}_xH_\eta,\varphi)|\le C_1\max_{V_\eta}|\varphi|,\quad |(\mathrm{div}_yH_\eta,\varphi)|\le C_2\max_{V_\eta}|\varphi| \tag{3.39}$$

for all $\varphi \in C_0^\infty(V_\eta)$. Since for all $\varphi \in C_0^\infty(V)$ the function $\check{\varphi}_\eta$ defined by

$$\check{\varphi}_\eta(x,y,t) = \varphi(x, y - \frac{x}{\eta}, t)$$

belongs to $C_0^\infty(V_\eta)$, we obtain from (3.39) that

$$\begin{aligned}
&|(\mathrm{div}_x\, \hat{H}_\eta, \varphi)| \\
&= \Big| \int_V H_\eta(x, \frac{x}{\eta} + y, t) \cdot \nabla_x\, \varphi(x,y,t)\, d(x,y,t) \Big| \\
&= \Big| \int_{V_\eta} H_\eta(x,y,t) \cdot \nabla_x\, \varphi(x,\xi,t)_{|_{\xi = y - \frac{x}{\eta}}}\, d(x,y,t) \Big| \\
&= \Big| \int_{V_\eta} H_\eta(x,y,t) \cdot \Big(\nabla_x\, \varphi(x, y - \frac{x}{\eta}, t) + \frac{1}{\eta} \nabla_y\, \varphi_\eta(x, y - \frac{x}{\eta}, t) \Big)\, d(x,y,t) \Big| \\
&\le \Big| \int_{V_\eta} H_\eta(x,y,t) \cdot \nabla_x\, \check{\varphi}_\eta(x,y,t) d(x,y,t) \Big| \\
&\qquad + \frac{1}{\eta} \Big| \int_{V_\eta} H_\eta(x,y,t) \cdot \nabla_y\, \check{\varphi}_\eta(x,y,t)\, d(x,y,t) \Big| \\
&\le (C_1 + \frac{1}{\eta} C_2)\, \max_{V_\eta} |\check{\varphi}_\eta| = (C_1 + \frac{1}{\eta} C_2)\, \max_V |\varphi|.
\end{aligned}$$

This estimate shows that $\mathrm{div}_x \hat{H}_\eta$ is a measure.

Consequently, by the Riesz representation theorem (cf. [26, pp. 49 and pp. 167]), to the total variation measure

$$\hat{\mu}_\eta = |\mathrm{div}_x \hat{H}_\eta| \tag{3.40}$$

there exists a $\hat{\mu}_\eta$–measurable function $\hat{\sigma}_\eta$ with

$$\mathrm{div}_x \hat{H}_\eta = \hat{\sigma}_\eta \hat{\mu}_\eta\,.$$

From this theorem it also follows that to the measure

$$\eta\, \mathrm{div}_x H_\eta + \mathrm{div}_y H_\eta$$

there exists a non-negative Radon measure μ_η and a μ_η–measurable function σ_η with

$$\eta\, \mathrm{div}_x H_\eta + \mathrm{div}_y H_\eta = \sigma_\eta \mu_\eta\,.$$

We call μ_η the total variation measure of $\eta\, \mathrm{div}_x H_\eta + \mathrm{div}_y H_\eta$ and write

$$|\eta\, \mathrm{div}_x H_\eta + \mathrm{div}_y H_\eta| = \mu_\eta\,. \tag{3.41}$$

Lemma 3.4 *For every $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+)$ we have*

$$\int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} \varphi(x, \frac{x}{\eta} + y, t)\, \eta\, d|\mathrm{div}_x \hat{H}_\eta| \tag{3.42}$$
$$= \int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} \varphi(x,y,t)\, d|\eta\, \mathrm{div}_x H_\eta + \mathrm{div}_y H_\eta|$$

and

$$\int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} \varphi(x, \frac{x}{\eta} + y, t)\, d\left|\frac{\partial}{\partial t}\hat{H}_\eta\right| = \int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} \varphi(x,y,t)\, d\left|\frac{\partial}{\partial t} H_\eta\right|. \tag{3.43}$$

Proof: Let $T : \Omega \times \mathbb{R}^3 \times \mathbb{R}^+ \to \Omega \times \mathbb{R}^3 \times \mathbb{R}^+$ be the map defined by

$$T(x,y,t) = (x, \frac{x}{\eta} + y, t)\,.$$

With the notations from (3.40) and (3.41), equation (3.42) can be written in the form

$$\int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} \varphi \circ T(x,y,t)\, \eta\, d\hat{\mu}_\eta = \int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} \varphi(x,y,t)\, d\mu_\eta\,. \tag{3.44}$$

This formula holds if $\mu_\eta = \eta T_* \hat{\mu}_\eta$, where the measure $T_* \hat{\mu}_\eta$ is defined by

$$T_* \hat{\mu}_\eta(A) = \hat{\mu}_\eta(T^{-1}(A))$$

for every measurable subset A. Since μ_η and $\eta T_* \hat{\mu}_\eta$ are Radon measures on $\Omega \times \mathbb{R}^3 \times \mathbb{R}^+$ and since Radon measures coincide if they coincide on open sets compactly contained in $\Omega \times \mathbb{R}^3 \times \mathbb{R}^+$, cf. [28, p. 62], equation (3.44) follows if we show that

$$\mu_\eta(V) = \eta T_* \hat{\mu}_\eta(V) = \eta \hat{\mu}_\eta(T^{-1}(V)) \tag{3.45}$$

for all open subsets V compactly contained in $\Omega \times \mathbb{R}^3 \times \mathbb{R}^+$. For such sets

$$\begin{aligned} \mu_\eta(V) &= \sup\Big\{ \int_V \varphi\, d(\eta\, \mathrm{div}_x H_\eta + \mathrm{div}_y H) \;\Big|\; \varphi \in C_0^\infty(V),\ |\varphi| \le 1 \Big\} \\ &= \sup\Big\{ -\int_V H_\eta(x,y,t) \cdot (\eta \nabla_x + \nabla_y)\varphi(x,y,t)\, d(x,y,t) \;\Big| \\ &\qquad\qquad \varphi \in C_0^\infty(V),\ |\varphi| \le 1 \Big\} \end{aligned} \tag{3.46}$$

and

$$\begin{aligned} \eta\hat{\mu}_\eta(T^{-1}(V)) &= \sup\Big\{ \int_{T^{-1}(V)} \varphi\, \eta\, d(\mathrm{div}_x \hat{H}_\eta) \;\Big|\; \varphi \in C_0^\infty(T^{-1}(V)),\ |\varphi| \le 1 \Big\} \\ &= \sup\Big\{ -\int_{T^{-1}(V)} \hat{H}_\eta(x,y,t) \cdot \eta\, \nabla_x\, \varphi(x,y,t)\, d(x,y,t) \;\Big| \\ &\qquad\qquad \varphi \in C_0^\infty(T^{-1}(V)),\ |\varphi| \le 1 \Big\}. \end{aligned} \tag{3.47}$$

Since $T^{-1}(x,y,t) = (x, y - \frac{x}{\eta}, t)$ and $|\det(T^{-1})'(x,y,t)| = 1$, we obtain

$$\begin{aligned}
&\int_{T^{-1}(V)} \hat{H}_\eta(x,y,t) \cdot \eta\, \nabla_x\, \varphi(x,y,t)\, d(x,y,t) \\
&= \int_{T^{-1}(V)} H_\eta(T(x,y,t)) \cdot \eta\, \nabla_x\, \varphi(x,y,t)\, d(x,y,t) \\
&= \int_V H_\eta(x,y,t) \cdot \eta\, \nabla_x\, \varphi(x,\xi,t)\big|_{\xi = y - \frac{x}{\eta}} d(x,y,t) \qquad (3.48) \\
&= \int_V H_\eta(x,y,t) \cdot (\eta\, \nabla_x + \nabla_y)\varphi(x, y - \frac{x}{\eta}, t)\, d(x,y,t) \\
&= \int_V H_\eta(x,y,t) \cdot (\eta\, \nabla_x + \nabla_y)(\varphi \circ T^{-1})(x,y,t)\, d(x,y,t)\,.
\end{aligned}$$

Since the mapping

$$\varphi \mapsto \varphi \circ T^{-1} : C_0^\infty(T^{-1}(V)) \to C_0^\infty(V)$$

is bijective, it follows from (3.48) that

$$\begin{aligned}
&\sup\Big\{ -\int_{T^{-1}(V)} \eta \hat{H}_\eta \cdot \nabla_x\, \varphi\, d(x,y,t) \;\Big|\; \varphi \in C_0^\infty(T^{-1}(V)),\ |\varphi| \le 1 \Big\} \\
&= \sup\Big\{ -\int_V H_\eta \cdot (\eta \nabla_x + \nabla_y)\varphi\, d(x,y,t) \;\Big|\; \varphi \in C_0^\infty(V),\ |\varphi| \le 1 \Big\}.
\end{aligned}$$

(3.45) results from this formula and from (3.46), (3.47). This proves (3.42). The proof of (3.43) runs exactly along the same lines, but is slightly simpler.

Definition 3.5 *For every $0 \le \eta < \eta_0$ let ν_η be a Radon measure on $\Omega \times \mathbb{R}^3 \times \mathbb{R}_0^+$. If*

$$\lim_{\eta \to 0} \int_{\Omega \times \mathbb{R}^3 \times \mathbb{R}^+} \varphi(x,y,t)\, d\nu_\eta = \int_{\Omega \times \mathbb{R}^3 \times \mathbb{R}^+} \varphi(x,y,t)\, d\nu_0 \qquad (3.49)$$

for all $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+)$, we write

$$\nu_\eta \overset{\infty}{\rightharpoonup} \nu_0\,.$$

If (3.49) *holds for all $\varphi \in C_0(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+)$, we write*

$$\nu_\eta \overset{*}{\rightharpoonup} \nu_0$$

and say that ν_η converges to ν_0 weak.*

Examples show that in general $\nu_\eta \overset{\infty}{\rightharpoonup} \nu_0$ does not imply $\nu_\eta \overset{*}{\rightharpoonup} \nu_0$. However, the following simple result holds:

Lemma 3.6 *Assume that for every open subset V compactly contained in $\Omega \times \mathbb{R}^3 \times \mathbb{R}^+$*

$$\sup_{\eta>0} |\nu_\eta|(V) < \infty.$$

Then $\nu_\eta \overset{\infty}{\rightharpoonup} \nu_0$ implies $\nu_\eta \overset{*}{\rightharpoonup} \nu_0$.

Proof: To $\varphi \in C_0(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+)$ choose an open set V with $\operatorname{supp}\varphi \subseteq V \subset\subset \Omega \times \mathbb{R}^3 \times \mathbb{R}^+$. To $\delta > 0$ we next choose a function $\chi \in C_0^\infty(V)$ with $\sup|\varphi - \chi| < \delta$. Then

$$\begin{aligned} |(\nu_\eta - \nu_0, \varphi)| &\le |(\nu_\eta - \nu_0, \chi)| + (|\nu_\eta| + |\nu_0|, |\varphi - \chi|) \\ &\le |(\nu_\eta - \nu_0, \chi)| + \delta(|\nu_0|(V) + \sup_{\eta>0} |\nu_\eta|(V)), \end{aligned}$$

from which the statement follows, since δ was arbitrary.

In Lemma 3.8 we give a criterion for the family $\{H_\eta\}_{0<\eta<\eta_0}$ which guarantees that

$$|\eta \operatorname{div}_x H_\eta + \operatorname{div}_y H_\eta| \overset{*}{\rightharpoonup} |\operatorname{div}_y H_0|,$$

with a suitable function H_0. This type of convergence is needed in the derivation of the homogenized evolution equation for the order parameter. In the proof of this lemma we rely on the following

Lemma 3.7 *Assume that V is a bounded open subset of $\mathbb{R}^n$ and that ν_η is a Radon measure on V for every $0 \le \eta < \eta_0$. If*

$$\nu_\eta \overset{*}{\rightharpoonup} \nu_0$$

and

$$|\nu_\eta|(V) \to |\nu_0|(V)$$

for $\eta \to 0$, then

$$|\nu_\eta| \overset{*}{\rightharpoonup} |\nu_0|.$$

A **proof** can be found in [75, pp. 141]. See also [32, pp. 9].

We assume that $H_\eta \in BV^{\mathrm{loc}}(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+)$ for all $0 \le \eta < \eta_0$ and that additionally for almost all (x,t) and all $0 \le \eta < \eta_0$ the functions

$$y \mapsto H_\eta(x,y,t)$$

are periodic with periodicity cell $Y \subseteq \mathbb{R}^3$. Without loss of generality we assume that the periodicity cell is the half open cube

$$Y = \{y = (y_1, y_2, y_3) \in \mathbb{R}^3 \mid 0 \le y_i < 1,\ i = 1,2,3\}.$$

For $\delta > 0$ we denote by

$$(\Omega \times \mathbb{R}^+)_\delta = \{(x,t) \in \Omega \times \mathbb{R}^+ \mid \operatorname{dist}((x,t), \partial(\Omega \times \mathbb{R}^+)) > \delta,\ |(x,t)| < \tfrac{1}{\delta}\}$$

the bounded open set of all points with distance from the boundary of $\Omega \times \mathbb{R}^+$ greater than δ and with norm less than $1/\delta$.

Lemma 3.8 *Assume that there exists a sequence $\{\Omega_m \times I_m\}_{m=1}^\infty$ of bounded open sets with*

$$(\Omega \times \mathbb{R}^+)_{\frac{1}{m}} \subseteq \Omega_m \times I_m \subseteq \Omega \times \mathbb{R}^+,$$

such that for all m

$$\lim_{\eta \to 0} \int_{\Omega_m \times Y \times I_m} |H_\eta(x,y,t) - H_0(x,y,t)|\, d(x,y,t) = 0. \tag{3.50}$$

$$\sup_{0<\eta<\eta_0} |\operatorname{div}_x H_\eta|(\Omega_m \times Y \times I_m) < \infty \tag{3.51}$$

$$\lim_{\eta \to 0} |\operatorname{div}_y H_\eta|(\Omega_m \times Y \times I_m) = |\operatorname{div}_y H_0|(\Omega_m \times Y \times I_m). \tag{3.52}$$

Then

$$|\eta \operatorname{div}_x H_\eta + \operatorname{div}_y H_\eta| \stackrel{*}{\rightharpoonup} |\operatorname{div}_y H_0|\,. \tag{3.53}$$

Proof: This statement results from Lemma 3.7. Therefore the main part of the proof consists in the verification of the assumptions of Lemma 3.7.

In the first step of the proof we construct a partition of unity on $\mathbb{R}^3$. We use the notations $s_+ = \max\{s, 0\}$ for $s \in \mathbb{R}$ and $|y|_\infty = \max_{1 \le i \le 3} |y_i|$ for $y = (y_1, y_2, y_3) \in \mathbb{R}^3$. Define a function $\chi \in C_0(\mathbb{R}^3, \mathbb{R}_0^+)$ by

$$\chi(y) = \prod_{i=1}^{3} (1 - |y_i|)_+\,, \quad y \in \mathbb{R}^3.$$

Then χ differs from zero only in the cube $\{y \in \mathbb{R}^3 \mid |y|_\infty \le 1\}$ consisting of 2^3 copies of Y. With this function we set $\chi_\alpha(x) = \chi(x - \alpha)$ and obtain a partition of unity $\{\chi_\alpha\}_{\alpha \in \mathbb{Z}_0^3}$ which satisfies for every positive integer m and every periodic function p with periodicity cell Y

$$\chi^{(m)}(x) = \sum_{|\alpha|_\infty \le m} \chi_\alpha(x) = 1, \quad |x|_\infty \le m, \tag{3.54}$$

$$\int_{\mathbb{R}^3} \chi^{(m)}(y) p(y) dy = (2m+1)^3 \int_Y p(y) dy. \tag{3.55}$$

For the proof of (3.55) note that the definition of $\chi^{(m)}$ in (3.54) yields

$$\int_{\mathbb{R}^3} \sum_{|\alpha|_\infty \le m} \chi_\alpha(y) p(y)\, dy = \int_{\mathbb{R}^2} \sum_{\alpha_2,\alpha_3=-m}^{m} \prod_{i=2}^{3} (1-|y_i-\alpha_i|)_+ \cdot \int_{\mathbb{R}} \sum_{\alpha_1=-m}^{m} (1-|y_1-\alpha_1|)_+ p(y)\, dy_1\, d(y_2,y_3)\,. \tag{3.56}$$

We use substitution and the periodicity of p to obtain

$$\begin{aligned}
&\sum_{\alpha_1=-m}^{m} \int_{\mathbb{R}} (1-|y_1-\alpha_1|)_+ p(y)\, dy_1 \\
&= \sum_{\alpha_1=-m}^{m} \int_{-1}^{1} (1-|y_1|)_+ p(y_1+\alpha_1, y_2, y_3)\, dy_1 \\
&= (2m+1)\Big(\int_0^1 (1-|y_1|) p(y)\, dy_1 + \int_0^1 (1-|\eta-1|) p(\eta-1, y_2, y_3)\, d\eta \Big) \\
&= (2m+1) \int_0^1 [(1-y_1) + (1-(1-y_1))] p(y)\, dy_1 = (2m+1) \int_0^1 p(y)\, dy_1\,.
\end{aligned}$$

Insertion of this formula into (3.56) and recursive application of it with the indices $i = 2, 3$ yields (3.55).

With the function $\chi^{(m)}$ just constructed the proof of the lemma is obtained as follows: For the measures $\nu_\eta^{(m)}(x,y,t) = \chi^{(m)}(y)\,(\eta \operatorname{div}_x H_\eta + \operatorname{div}_y H_\eta)(x,y,t)$, $\eta \ge 0$, we prove that

$$\nu_\eta^{(m)} \overset{\infty}{\rightharpoonup} \nu_0^{(m)} \tag{3.57}$$

and

$$\lim_{\eta\to 0} |\nu_\eta^{(m)}|(\Omega_m \times \mathbb{R}^3 \times I_m) = |\nu_0^{(m)}|(\Omega_m \times \mathbb{R}^3 \times I_m), \tag{3.58}$$

for all $m \in \mathbb{N}$. Since to any open set V compactly contained in $\Omega \times \mathbb{R}^3 \times \mathbb{R}^+$ there exists m with

$$V \subseteq \{(x,y,t) \mid (x,t) \in (\Omega \times \mathbb{R}^+)_{\frac{1}{m}},\ y \in \mathbb{R}^3\} \subseteq \Omega_m \times \mathbb{R}^3 \times I_m\,,$$

it follows from (3.58) that

$$\sup_{\eta>0} |\nu_\eta^{(m)}|(V) < \infty.$$

This relation, (3.57) and Lemma 3.6 together imply

$$\nu_\eta^{(m)} \overset{*}{\rightharpoonup} \nu_0^{(m)}\,,$$

and this result, (3.58) and Lemma 3.7 yield

$$|\nu_\eta^{(m)}| \overset{*}{\rightharpoonup} |\nu_0^{(m)}|$$

on the set $\Omega_m \times \mathbb{R}^3 \times I_m$ for all m. Note that the unbounded set $\Omega_m \times \mathbb{R}^3 \times I_m$ can be inserted for the bounded set V in Lemma 3.7, since the measure $\nu_\eta^{(m)}$ restricted to the set $\Omega_m \times \mathbb{R}^3 \times I_m$ has bounded support. The statement of Lemma 3.8 is an immediate consequence of this result, since (3.54) implies that to any $\varphi \in C_0(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+)$ there exists m with $\operatorname{supp}\varphi \subseteq \Omega_m \times \{y \mid \chi^{(m)} = 1\} \times I_m$.

To complete the proof it remains to show (3.57) and (3.58). For the proof of (3.57) let $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+)$ and choose m with $\operatorname{supp}\varphi \subseteq \Omega_m \times \mathbb{R}^3 \times I_m$. Using that the functions $\varphi^{(m)}(x,y,t) = \chi^{(m)}(y)\varphi(x,y,t)$ and $\varphi_\alpha(x,y,t) = \chi_\alpha(y)\varphi(x,y,t)$ have weak derivatives in L^∞, we obtain

$$\begin{aligned}
&\Big| \int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} \varphi(x,y,t)\chi^{(m)}(y)\Big(d(\eta \operatorname{div}_x H_\eta + \operatorname{div}_y H_\eta) - d(\operatorname{div}_y H_0)\Big)\Big| = \\
&= \Big| - \int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} H_\eta(x,y,t) \cdot \eta \nabla_x \varphi^{(m)}(x,y,t)\, d(x,y,t) \\
&\qquad - \int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} (H_\eta(x,y,t) - H_0(x,y,t)) \cdot \nabla_y \varphi^{(m)}(x,y,t)\, d(x,y,t)\Big| \\
&\le \sum_{|\alpha|_\infty \le m} \Big(\int_{\Omega_m \times \operatorname{supp}\chi_\alpha \times I_m} \eta |H_\eta(x,y,t)|\, |\nabla_x \varphi_\alpha(x,y,t)|\, d(x,y,t) \\
&\quad + \int_{\Omega_m \times \operatorname{supp}\chi_\alpha \times I_m} |H_\eta(x,y,t) - H_0(x,y,t)|\, |\nabla_y \varphi_\alpha(x,y,t)|\, d(x,y,t)\Big) \\
&\le \sum_{|\alpha|_\infty \le m} \Big(\max |\nabla_x \varphi_\alpha(x,y,t)| + \max |\nabla_y \varphi_\alpha(x,y,t)|\Big) \\
&\quad \cdot 2^3 \int_{\Omega_m \times Y \times I_m} \Big(\eta |H_\eta(x,y,t)| + |H_\eta(x,y,t) - H_0(x,y,t)|\Big)\, d(x,y,t) \to 0
\end{aligned}$$

for $\eta \to 0$. To get the last inequality sign we used that the cube $\operatorname{supp}\chi_\alpha$ consists of 2^3 copies of Y, and we applied the periodicity of H_η. The convergence to zero is implied by (3.50) and by

$$\sup_{\eta_0 > \eta > 0} \int_{\Omega_m \times Y \times I_m} |H_\eta(x,y,t)|\, d(x,y,t) < \infty\,,$$

which also is a consequence of (3.50). This proves (3.57).

To verify (3.58) we note that the equation (3.55) yields for the measures $|\nu_\eta^{(m)}|$ by some straightforward considerations

$$|\nu_\eta^{(m)}|(\Omega_m \times \mathbb{R}^3 \times I_m) = (2m+1)^3 |\nu_\eta|(\Omega_m \times Y \times I_m),$$

for all $\eta \geq 0$. Here the measures ν_η are defined by $\nu_\eta = \eta \operatorname{div}_x H_\eta + \operatorname{div}_y H_\eta$. Therefore, to prove (3.58) it suffices to show that

$$\lim_{\eta \to 0} |\nu_\eta|(\Omega_m \times Y \times I_m) = |\nu_0|(\Omega_m \times Y \times I_m). \tag{3.59}$$

To verify this relation, note that the inverse triangle inequality and (3.51) imply

$$\begin{aligned} \Big| |\eta \operatorname{div}_x H_\eta + \operatorname{div}_y H_\eta|(\Omega_m \times Y \times I_m) - |\operatorname{div}_y H_\eta|(\Omega_m \times Y \times I_m)\Big| \\ \leq |\eta \operatorname{div}_x H_\eta|(\Omega_m \times Y \times I_m) \leq \eta C. \end{aligned}$$

From the hypothesis (3.52) we thus obtain

$$\begin{aligned} &\Big| |\nu_\eta|(\Omega_m \times Y \times I_m) - |\nu_0|(\Omega_m \times Y \times I_m)\Big| \\ &\leq \Big| |\eta \operatorname{div}_x H_\eta + \operatorname{div}_y H_\eta|(\Omega_m \times Y \times I_m) - |\operatorname{div}_y H_\eta|(\Omega_m \times Y \times I_m)\Big| \\ &\qquad + \Big| |\operatorname{div}_y H_\eta|(\Omega_m \times Y \times I_m) - |\operatorname{div}_y H_0|(\Omega_m \times Y \times I_m)\Big| \\ &\leq \eta C + \Big| |\operatorname{div}_y H_\eta|(\Omega_m \times Y \times I_m) - |\operatorname{div}_y H_0|(\Omega_m \times Y \times I_m)\Big| \to 0 \end{aligned}$$

for $\eta \to 0$. Therefore (3.59) and also (3.58) hold. This completes the proof of the lemma.

3.4 Homogenized evolution equation for the order parameter and homogenized initial-boundary value problem

To derive the homogenized form of the equation (3.4) we must insert the functions $\hat{u}_\eta$, $\hat{T}_\eta$, $\hat{z}_\eta$, $\hat{S}_\eta$ from (3.12) into (3.4) and study the limits of the terms on both sides of the equation for $\eta \to 0$. These are limits in the distribution sense. Therefore, to study these limits we must generalize Definition 3.1 and introduce a *family of distribution solutions of the initial-boundary value problem depending on the fast variable.* We begin with this definition.

The space $BV^{\mathrm{loc}}(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+)$ and the total variation measure was introduced before Lemma 2.3. In the following definition we also need the space $BV^{\mathrm{loc}}(\Omega \times \mathbb{R}^3 \times \mathbb{R}_0^+)$, which consists of all functions w on $\Omega \times \mathbb{R}^3 \times \mathbb{R}_0^+$ with the property that for every open set V compactly contained in $\Omega \times \mathbb{R}^3 \times \mathbb{R}$ the restriction of w to $V \cap (\Omega \times \mathbb{R}^3 \times \mathbb{R}^+)$ satisfies

$$w|_{V\cap(\Omega\times\mathbb{R}^3\times\mathbb{R}^+)} \in BV(V \cap (\Omega \times \mathbb{R}^3 \times \mathbb{R}^+))\,.$$

For the given initial data $z_0^{(0)} : \Omega \times \mathbb{R}^3 \to \mathbb{R}^N$ and $S_0^{(0)} : \Omega \times \mathbb{R}^3 \to \{0, 1\}$ we assume as above that $y \mapsto z_0^{(0)}(x, y)$ and $y \mapsto S_0^{(0)}(x, y)$ are periodic with periodicity cell Y and that this periodicity cell satisfies (3.10).

In the equation (3.4), which was derived in Lemma 2.4 for piecewise continuously differentiable z, the derivatives $\nabla_x z$ are the classical derivatives on $(\Omega \times \mathbb{R}^+)\backslash\Gamma$ and differ from the distributional derivatives by a measure on Γ generated by jumps of z across Γ. To avoid regularity problems, we want to use in the following definition only weak or distributional derivatives. $\nabla_x z$ could be computed from the distributional derivatives by subtraction of the measure on the interface Γ. Since we also want to avoid the discussion of the regularity of Γ, which would be necessary if this measure would explicitely appear in the definition, we require in the following definition of a family of distribution solutions depending on the fast variable that z is continuous across the interface. This means that we take the identity for the function g in the interface condition (3.6). In this case the weak and the classical derivatives coincide when the latter exist, and for $\nabla_x z$ in (3.4) we can insert the weak derivatives. Also for $\nabla_x u$ we can take the weak derivatives, since in all our investigations we assume that u is continuous across Γ.

Definition 3.9 a.) *Let $z_0^{(0)} \in L^{1,\mathrm{loc}}(\Omega \times \mathbb{R}^3)$, let $S_0^{(0)}$ be measurable and let $\eta > 0$ be constant. The function (u, T, z, S) is a distribution solution of the partial differential equations*

$$\begin{aligned}
-\mathrm{div}_x\, T(x, y, t) &= b(x, t) && (3.60)\\
T(x, y, t) &= D(S(x, y, t))(\varepsilon(\nabla_x u(x, y, t)) - \varepsilon^*(S(x, y, t)) \\
&\qquad\qquad - Bz(x, y, t)) && (3.61)\\
z_t(x, y, t) &= f(S(x, y, t), T(x, y, t), z(x, y, t)) && (3.62)\\
|S_t(x, y, t)| &= \eta c|\mathrm{div}_x\, C(\nabla_x u, S, z) && (3.63)\\
&\quad -\rho(\nabla_x z)^T \nabla_z \psi(\varepsilon(\nabla_x u), S, z) - (\nabla_x u)^T b|
\end{aligned}$$

defined for $(x, y, t) \in \Omega \times \mathbb{R}^3 \times \mathbb{R}^+$, of the interface conditions

$$[u(x, y, t)] = [T(x, y, t)]n(x) = [z(x, y, t)] = 0, \quad (x, y) \in \Gamma(t),\ t \in \mathbb{R}^+, \quad (3.64)$$

of the boundary condition

$$T(x, y, t)n(x) = 0\,, \quad (x, y, t) \in \partial\Omega \times \mathbb{R}^3 \times \mathbb{R}_0^+\,, \quad (3.65)$$

and of the initial conditions

$$\left.\begin{aligned} z(x,y,0) &= z_0^{(0)}(x, \frac{x}{\eta} + y), \\ S(x,y,0) &= S_0^{(0)}(x, \frac{x}{\eta} + y), \end{aligned}\right\} \quad (x,y) \in \Omega \times \mathbb{R}^3\,, \tag{3.66}$$

if the following conditions (i)–(v) *are satisfied:*

(i) *The functions* $u,\ T,\ z,\ S,\ C,\ f$ *and* b *satisfy*

$$\begin{aligned} S,\ C(\nabla_x u, S, z) &\in BV^{\mathrm{loc}}(\Omega \times \mathbb{R}^3 \times \mathbb{R}_0^+) \\ u,\ \nabla_x u,\ \nabla_x z, &\in L^{1,\mathrm{loc}}(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+) \\ T,\ b &\in L^{1,\mathrm{loc}}(\overline{\Omega} \times \mathbb{R}^3 \times \mathbb{R}^+) \\ z,\ f(S,T,z) &\in L^{1,\mathrm{loc}}(\Omega \times \mathbb{R}^3 \times \mathbb{R}_0^+), \end{aligned}$$

and also

$$(\nabla_x u)^T b,\ (\nabla_x z)^T \nabla_z \psi(\varepsilon(\nabla_x u), S, z) \in L^{1,\mathrm{loc}}(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+)$$

(ii) *The equation*

$$(T, \nabla_x \varphi) = (b, \varphi), \tag{3.67}$$

holds for all $\varphi \in C_0^\infty(\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^+, \mathbb{R}^3)$, *the equation* (3.61) *holds for almost all* $(x,y,t) \in \Omega \times \mathbb{R}^3 \times \mathbb{R}^+$, *and the equation*

$$\begin{aligned} -(z, \varphi_t) &= (f(S,T,z), \varphi) \\ &\quad + \int_{\Omega\times\mathbb{R}^3} z_0^{(0)}(x, \frac{x}{\eta} + y) \cdot \varphi(x,y,0)\, d(x,y), \end{aligned} \tag{3.68}$$

is satisfied for all $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^3 \times \mathbb{R}, \mathbb{R}^N)$

(iii) *The equation* (3.63) *holds in the sense of measures, where the absolute values on both sides of this equation denote the total variation measures*

(iv) *The interface condition*

$$[u(x,y,t)] = 0 \tag{3.69}$$

holds for almost all $(x,y) \in \Gamma(t) \times \mathbb{R}^3,\ t \in \mathbb{R}^+$

(v) *The initial condition*

$$S(x,y,0) = S_0^{(0)}(x, \frac{x}{\eta} + y) \tag{3.70}$$

holds for almost all $(x,y) \in \Omega \times \mathbb{R}^3$.

b.) *We say, that the distribution solution* (u, T, z, S) *of* (3.60)–(3.66) *defines a family of distribution solutions of the initial-boundary value problem* (3.1)–(3.4), (3.6), (3.7), (3.11) *depending on the fast variable* y *with parameter* η *and initial data* $(z_0^{(0)}, S_0^{(0)})$.

Of course, the equation (3.67) combines the equation (3.60), the interface condition for T and the boundary condition (3.65), the equation (3.68) combines the equation (3.62), the interface condition for z and the first one of the initial conditions (3.66), and in (3.70) we use that as a BV-function S has a trace on the part $\Omega \times \mathbb{R}^3 \times \{0\}$ of the boundary of $\Omega \times \mathbb{R}^3 \times \mathbb{R}^+$.

Now we derive the homogenized evolution equation for the order parameter S. For $0 < \eta < \eta_0$ let $(\hat{u}_\eta, \hat{T}_\eta, \hat{z}_\eta, \hat{S}_\eta)$ be a family of distribution solutions of the initial-boundary value problem depending on the fast variable with parameter η, which can be represented in the form (3.12)–(3.16). Let C denote the Eshelby tensor and ψ the free energy. We define

$$\begin{aligned}
\hat{C}_\eta(x, y, t) &= C(\nabla_x \hat{u}_\eta(x, y, t), \hat{S}_\eta(x, y, t), \hat{z}_\eta(x, y, t)), \\
\nabla_z \hat{\psi}_\eta(x, y, t) &= \nabla_z \psi(\varepsilon(\nabla_x \hat{u}_\eta(x, y, t)), \hat{S}_\eta(x, y, t), \hat{z}_\eta(x, y, t))
\end{aligned}$$

and

$$\begin{aligned}
C_\eta(x, y, t) &= C(\nabla_x u_\eta(x, y, t) + \frac{1}{\eta} \nabla_y u_\eta(x, y, t), S_\eta(x, y, t), z_\eta(x, y, t)), \\
\nabla_z \psi_\eta(x, y, t) &= \\
&= \nabla_z \psi(\varepsilon(\nabla_x u_\eta(x, y, t)) + \frac{1}{\eta} \varepsilon(\nabla_y u_\eta(x, y, t)), S_\eta(x, y, t), z_\eta(x, y, t)),
\end{aligned}$$

hence

$$\hat{C}_\eta(x, y, t) = C_\eta(x, \frac{x}{\eta} + y, t), \quad \nabla_z \hat{\psi}_\eta(x, y, t) = \nabla_z \psi_\eta(x, \frac{x}{\eta} + y, t).$$

Under suitable boundedness conditions for the function u_2 in (3.13) and its derivatives, we have

$$\nabla_x u_\eta(x, y, t) + \frac{1}{\eta} \nabla_y u_\eta(x, y, t) \to \nabla_x u_0(x, t) + \nabla_y u_1(x, y, t)$$

for $\eta \to 0$. Therefore we assume below that for $\eta \to 0$ the function C_η tends to the function

$$C_0(x, y, t) = C(\nabla_x u_0(x, t) + \nabla_y u_1(x, y, t), S_0(x, y, t), z_0(x, y, t)),$$

and $\nabla_z \psi_\eta$ tends to

$$\nabla_z \psi_0(x, y, t) = \nabla_z \psi(\varepsilon(\nabla_x u_0(x, t)) + \varepsilon(\nabla_y u_1(x, y, t)), S_0(x, y, t), z_0(x, y, t)) \,.$$

With these definitions we can write the equation which results from insertion of $(\hat{u}_\eta, \hat{T}_\eta, \hat{z}_\eta, \hat{S}_\eta)$ into the evolution equation (3.63) in the form

$$\begin{aligned} \Big| \frac{\partial}{\partial t}\hat{S}_\eta(x,y,t) \Big| \quad = \quad \eta c \Big| & \operatorname{div}_x \hat{C}_\eta(x,y,t) \\ & - \rho(\nabla_x \hat{z}_\eta(x,y,t))^T \nabla_z \hat{\psi}_\eta(x,y,t) \\ & - (\nabla_x \hat{u}_\eta(x,y,t))^T b(x,t) \Big|. \end{aligned} \tag{3.71}$$

Lemma 3.10 *Assume that*

$$\operatorname{div}_x \hat{C}_\eta - \rho(\nabla_x \hat{z}_\eta)^T \nabla_z \hat{\psi}_\eta - (\nabla_x \hat{u}_\eta)^T b$$

and $\frac{\partial}{\partial t}\hat{S}_\eta$ *are measures, and that the corresponding total variation measures satisfy* (3.71). *Assume moreover that*

$$\Big|\frac{\partial}{\partial t}S_\eta\Big| \stackrel{*}{\rightharpoonup} \Big|\frac{\partial}{\partial t}S_0\Big| \tag{3.72}$$

and

$$\begin{aligned} & \Big|\eta \operatorname{div}_x C_\eta + \operatorname{div}_y C_\eta - \rho(\eta\nabla_x z_\eta + \nabla_y z_\eta)^T \nabla_z \psi_\eta - (\eta\nabla_x u_\eta + \nabla_y u_\eta)^T b\Big| \\ & \stackrel{*}{\rightharpoonup} \Big|\operatorname{div}_y C_0 - \rho(\nabla_y z_0)^T \nabla_z \psi_0\Big| \end{aligned} \tag{3.73}$$

for $\eta \to 0$. *Then the equation*

$$\Big|\frac{\partial}{\partial t}S_0(x,y,t)\Big| = c\Big|\operatorname{div}_y C_0(x,y,t) - \rho(\nabla_y z_0(x,y,t))^T \nabla_z \psi_0(x,y,t)\Big| \tag{3.74}$$

holds in the sense of measures on $\Omega \times \mathbb{R}^3 \times \mathbb{R}^+$.

Remark. Equation (3.74) is the homogenized evolution equation for the order parameter. Because of the nonlinear dependence of C and $\rho(\nabla_x z)^T \nabla_z \psi$ on (u,T,z,S), it is clear that weak convergence of $(u_\eta, T_\eta, z_\eta, S_\eta)$ to (u_0, T_0, z_0, S_0) is not sufficient to guarantee (3.73). This problem arises in all investigations of nonlinear partial differential equations and in particular in investigations of quasilinear hyperbolic conservation laws. In the present problem an additional difficulty is introduced through the presence of the total variation measure. We do not investigate this problem any further, but only refer to the criterion for weak convergence of total variation measures given in Lemma 3.8.

Proof: If we insert the function S for H in the equation (3.43) of the Lemma 3.4, we obtain for every $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+, \mathbb{R})$ that

$$\int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} \varphi(x, \frac{x}{\eta} + y, t)\, d\Big|\frac{\partial}{\partial t}\hat{S}_\eta\Big| = \int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} \varphi(x,y,t)\, d\Big|\frac{\partial}{\partial t}S_\eta\Big|. \tag{3.75}$$

Insertion of C for H in (3.42) yields a corresponding result for the measures $|\mathrm{div}_x \hat{C}_\eta|$ and $|\eta \mathrm{div}_x C_\eta + \mathrm{div}_y C_\eta|$. Examination of the proof of (3.42) shows that the result can be extended to the measure on the right hand side of (3.71) and that the same proof yields for all $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+)$

$$\begin{aligned}
&\int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} \varphi(x, \frac{x}{\eta} + y, t)\eta \, d\Big|\mathrm{div}_x \hat{C}_\eta - \rho(\nabla_x \hat{z}_\eta)^T \nabla_z \hat{\psi}_\eta - (\nabla_x \hat{u}_\eta)^T b\Big| \\
&= \int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} \varphi(x, y, t) \, d\Big|\eta \mathrm{div}_x C_\eta + \mathrm{div}_y C_\eta - \rho(\eta\nabla_x z_\eta + \nabla_y z_\eta)^T \nabla_z \psi_\eta \\
&\qquad\qquad - (\eta\nabla_x u_\eta + \nabla_y u_\eta)^T b\Big| . \qquad (3.76)
\end{aligned}$$

From (3.71), (3.75) and (3.76) we thus obtain

$$\begin{aligned}
&\int_{\Omega\times\mathbb{R}^3\times\mathbb{R}^+} \varphi(x, y, t) \left(d\Big|\frac{\partial}{\partial t} S_\eta\Big| - c\,\Big|\eta \mathrm{div}_x C_\eta + \mathrm{div}_y C_\eta \right. \\
&\qquad \left. - \rho(\eta\nabla_x z_\eta + \nabla_y z_\eta)^T \nabla_z \psi_\eta - (\eta\nabla_x u_\eta + \nabla_y u_\eta)^T b\Big| \right) = 0
\end{aligned}$$

for all $\varphi \in C_0^\infty(\Omega \times \mathbb{R}^3 \times \mathbb{R}^+, \mathbb{R})$, which implies

$$\begin{aligned}
\Big|\frac{\partial}{\partial t} S_\eta\Big| &= c\,\Big|\eta \mathrm{div}_x C_\eta + \mathrm{div}_y C_\eta - \rho(\eta\nabla_x z_\eta + \nabla_y z_\eta)^T \nabla_z \psi_\eta \\
&\qquad - (\eta\nabla_x u_\eta + \nabla_y u_\eta)^T b\Big| .
\end{aligned}$$

By (3.72) and (3.73), the left hand side tends to $|\frac{\partial}{\partial t} S_0|$ and the right hand side tends to $c|\mathrm{div}_y C_0 - \rho(\nabla_y z_0)^T \nabla_z \psi_0|$. Therefore these limits must coincide, which proves (3.74).

Next we define the homogenized initial-boundary value problem. In this definition the *mean stress*

$$T_\infty(x, t) = M_Y T_0(x, \cdot, t) = \int_Y T_0(x, y, t)\, dy$$

playes an important part:

Definition 3.11 *The homogenized initial-boundary value problem associated to the initial-boundary value problem* (3.1)–(3.4), (3.6)–(3.8) *is constituted by the equations*

$$-\mathrm{div}_x T_\infty(x, t) = b(x, t), \qquad (3.77)$$

$$T_\infty(x, t) = \mathcal{F}_{s\le t}(\nabla_x u_0(x, s), x), \qquad (3.78)$$

$$T_\infty(x, t) n(x) = 0, \quad x \in \partial\Omega, \quad t \ge 0. \qquad (3.79)$$

Here the history functional $\nabla_x u_0(x,\cdot) \mapsto T_\infty(x,\cdot) = \mathcal{F}_{s\le t}(\nabla_x u_0(x,s),x)$ *is defined by the equation*

$$T_\infty(x,t) = M_Y T_0(x,\cdot,t), \tag{3.80}$$

which couples the mean stress to the micro stress T_0 *, and by an initial-boundary value problem in the* representative volume element*, which defines* T_0 *and which consists of the four equations*

$$\begin{aligned}
&-D(S_0(x,\cdot,t))\varepsilon(\nabla_y u_1(x,\cdot,t)) = && (3.81)\\
&\quad = P^\perp_{(S_0,x,t)}\{D(S_0(x,\cdot,t))(\varepsilon(\nabla_x u_0(x,t)) - \varepsilon^*(S_0(x,\cdot,t)) - Bz_0(x,\cdot,t))\},\\
&T_0(x,\cdot,t) = && (3.82)\\
&\quad = P_{(S_0,x,t)}\{D(S_0(x,\cdot,t))(\varepsilon(\nabla_x u_0(x,t)) - \varepsilon^*(S_0(x,\cdot,t)) - Bz_0(x,\cdot,t))\},\\
&\frac{\partial}{\partial t} z_0(x,y,t) \;=\; f(S_0(x,y,t),T_0(x,y,t),z_0(x,y,t)), && (3.83)\\
&\Big|\frac{\partial}{\partial t} S_0\Big| \;=\; c\Big|\operatorname{div}_y C(\nabla_x u_0 + \nabla_y u_1, S_0, z_0) && (3.84)\\
&\qquad - \rho(\nabla_y z_0)^T \nabla_z \psi(\varepsilon(\nabla_x u_0 + \nabla_y u_1), S_0, z_0)\Big|,
\end{aligned}$$

where $P^\perp_{(S_0,x,t)} = (I - P_{(S_0,x,t)}) : L^2(Y) \to \mathcal{D}_0^\perp \subseteq L^2(Y)$ *is the orthogonal projector onto the orthogonal space* $\mathcal{D}_0^\perp$ *of* $\mathcal{D}_0$ *,*
of the interface conditions

$$[u_0(x,y,t)] = [T_0(x,y,t)]n(x,t) = [z_0(x,y,t)] = 0, \quad (x,y,t) \in \Gamma, \tag{3.85}$$

of the boundary condition

$$y \mapsto (u_1(x,y,t), T_0(x,y,t), z_0(x,y,t), S_0(x,y,t)) \tag{3.86}$$

has periodicity cell Y*,*

and of the initial conditions

$$z_0(x,y,0) = z_0^{(0)}(x,y), \quad S_0(x,y,0) = S_0^{(0)}(x,y), \quad (x,y) \in \Omega \times \mathbb{R}^3. \tag{3.87}$$

Scholia. *1.* For every fixed $x \in \Omega$ the equations (3.81)–(3.87) define an initial-boundary value problem in the domain $Y \times \mathbb{R}^+$ for the unknown function $(y,t) \mapsto (u_1,T_0,S_0,z_0)(x,y,t)$, which has the same form as the initial-boundary value problem (3.1)–(3.8). This is hidden by the introduction of the projections $P_{(S_0,x,t)}$ and $(I - P_{(S_0,x,t)})$.

To see that (3.81)–(3.87) has this form, note that the pair of equations (3.81) and (3.82) is equivalent to the pair of equations (3.26) and (3.34).

In fact, at the end of the proof of Theorem 3.2 it was shown that (3.26) and (3.34) imply the equations (3.35) and (3.24), which coincide with (3.81) and (3.82). Conversely, (3.26) is obtained from (3.82), since $P_{(S_0,x,t)}$ is a projector to the space $\mathcal{D}_0$ of periodic functions with vanishing divergence, and (3.34) is obtained from (3.81) and (3.82) by addition of these two equations. Therefore the equations (3.81) and (3.82) can be replaced by

$$\operatorname{div}_y T_0(x,y,t) = 0, \tag{3.88}$$

$$\begin{aligned} T_0(x,y,t) &= D(S_0(x,y,t))\Big(\varepsilon(\nabla_x u_0(x,t) + \nabla_y u_1(x,y,t)) \\ &\qquad - \varepsilon^*(S_0(x,y,t)) - Bz_0(x,y,t)\Big), \end{aligned} \tag{3.89}$$

and the problem constituted by these two equations and by (3.83)–(3.87) is of the form of (3.1)–(3.8). The main difference is the presence of the term

$$\nabla_x u_0(x,t)$$

in (3.89) and in (3.84), which from the point of view of the initial-boundary value problem (3.88), (3.89), (3.83)–(3.87) is a given function. This term imposes a deformation field on the representative volume element, which does not depend on y. Hence, for every given time this deformation field is constant throughout the representative volume element Y. Besides the micro stress T_0 also u_1 is determined by this initial-boundary value problem. The function u_1 playes the part of a micro displacement.

2. The periodicity requirement for u_1 and T_0 in the boundary condition (3.86) is not needed in conjunction with the equations (3.81) and (3.82), since it is a consequence of the definition of the projection $P_{(S_0,x,t)}$. It is needed, however, in conjunction with the equations (3.88) and (3.89).

3. The x–dependence of the history functional $\mathcal{F}_{s\le t}(\nabla_x u_0(x,s),x)$ is introduced by the x–dependence of the initial data $z_0^{(0)}(x,y)$ and $S_0^{(0)}(x,y)$.

4. By a formal reasoning, from the boundary condition (3.65) one would obtain the boundary condition

$$T_0(x,y,t)n(x) = 0, \quad (x,y,t) \in \partial\Omega \times \mathbb{R}^3 \times \mathbb{R}_0^+$$

for the homogenized problem, which is stronger than the boundary condition (3.79). However, in accordance with well known results from the theory of homogenization for linear elliptic problems, cf. [7, pp. 87], one expects that this stronger boundary condition cannot be imposed in the homogenized problem and that (3.79) is the right condition.

5. The functions u_0, u_1, T_0, z_0 and S_0 determined as solution of the homogenized initial-boundary value problem can be used in two ways:

Since these functions are the leading terms in the expansions (3.13)–(3.16), the functions

$$\hat{u}_{0,\eta}(x,y,t) = u_0(x,t) + \eta u_1(x, \frac{x}{\eta} + y, t), \tag{3.90}$$

$$\hat{T}_{0,\eta}(x,y,t) = T_0(x, \frac{x}{\eta} + y, t),$$

$$\hat{z}_{0,\eta}(x,y,t) = z_0(x, \frac{x}{\eta} + y, t),$$

$$\hat{S}_{0,\eta}(x,y,t) = S_0(x, \frac{x}{\eta} + y, t),$$

form an asymptotic approximation to the solution $(\hat{u}_\eta, \hat{T}_\eta, \hat{z}_\eta, \hat{S}_\eta)$ of the microscopic initial-boundary value problem (3.1)–(3.7), (3.11):

$$(\hat{u}_\eta, \hat{T}_\eta, \hat{z}_\eta, \hat{S}_\eta) - (\hat{u}_{0,\eta}, \hat{T}_{0,\eta}, \hat{z}_{0,\eta}, \hat{S}_{0,\eta}) \to 0 \tag{3.91}$$

for $\eta \to 0$. This is the first usage.

For the second usage we define the mean stress $\hat{T}_{\eta,\infty}$ of the exact solution in the cell $\eta Y = \{\eta y \mid y \in Y\}$ by

$$\begin{aligned}
\hat{T}_{\eta,\infty}(x,y,t) &= \frac{1}{|\eta Y|} \int_{\eta Y} \hat{T}_\eta(x+z, y, t)\, dz \\
= \frac{1}{|\eta Y|} \int_{\eta Y} T_\eta(x+z, \frac{x+z}{\eta} + y, t)\, dz &= \frac{1}{|\eta Y|} \int_{\eta Y} T_\eta(x+z, \frac{x+z}{\eta}, t)\, dz,
\end{aligned}$$

where $|\eta Y| = \int_{\eta Y} dy$. Here we used (3.12) and the periodicity of T_η. This computation shows that $\hat{T}_{\eta,\infty}(x,y,t) = \hat{T}_{\eta,\infty}(x,t)$. We also use that

$$\begin{aligned}
T_\infty(x,t) &= \int_Y T_0(x,y,t)\, dy = \int_Y T_0(x, \frac{x}{\eta} + y, t)\, dy \\
&= \frac{1}{|\eta Y|} \int_{\eta Y} T_0(x, \frac{x+y}{\eta}, t)\, dy \\
&= \frac{1}{|\eta Y|} \int_{\eta Y} T_0(x+y, \frac{x+y}{\eta}, t)\, dy + r(\eta),
\end{aligned}$$

with the remainder

$$r(\eta) = \frac{1}{|\eta Y|} \int_{\eta Y} \Big(T_0(x, \frac{x+y}{\eta}, t) - T_0(x+y, \frac{x+y}{\eta}, t) \Big)\, dy \to 0$$

for $\eta \to 0$. From (3.91) we thus have

$$
\begin{aligned}
&|\hat{T}_{\eta,\infty}(x,t) - T_\infty(x,t)| \\
&\le \Big| \frac{1}{|\eta Y|} \int_{\eta Y} \Big(T_\eta(x+y, \frac{x+y}{\eta}, t) - T_0(x+y, \frac{x+y}{\eta}, t) \Big)\, dy \Big| + r(\eta) \to 0
\end{aligned}
$$

for $\eta \to 0$. As second usage we therefore see from this relation and from (3.90), (3.91) that u_0 and T_∞, which are macroscopic, non-oscillating quantities, are the limits of the displacement $\hat{u}_\eta$ and of the averaged stress $\hat{T}_{\eta,\infty}$ over the cell ηY for $\eta \to 0$:

$$
(\hat{u}_\eta, \hat{T}_{\eta,\infty}) \to (u_0, T_\infty).
$$

6. The history functional $\mathcal{F}_{s\le t}(\nabla_x u_0(x,s), x)$ has the input function $s \mapsto \nabla_x u_0(x,s)$ and the output function $t \mapsto T_\infty(x,t)$. To compute $T_\infty(x,\cdot)$ from the deformation gradient $\nabla_x u_0(x,\cdot)$ for a given fixed x, this deformation gradient is considered as a function $(y,s) \mapsto \nabla_x u_0(x,s)$ constant with respect to y, which we insert in the initial-boundary value problem (3.88), (3.89), (3.83)–(3.87) posed in the representative volume element Y. Then the functions u_1, T_0, S_0, z_0 varying with respect to y in the representative volume element are computed by solving this initial-boundary value problem. Finally, we obtain the y–independent value $T_\infty(x,t)$ by taking the mean value of $T_0(x,\cdot,t)$ over the representative volume element. This computation of the y–independent function T_∞ from the y–independent function $\nabla_x u_0$ via the determination of y–dependent functions as solutions of an initial-boundary value problem is computationally expensive. An important open problem is therefore to devise a method to eliminate the y–variable by homogenization of the initial-boundary value problem (3.88), (3.89), (3.83)–(3.87) posed in the representative volume element. The homogenization procedure discussed in this article can therefore only be considered as a first step. The homogenization of the microscopic initial-boundary value problem leading to a history functional defined by an initial-boundary value problem in the representative volume element should be completed by a homogenization procedure, which replaces this initial-boundary value problem in the representative volume element by a constitutive relation, which for every x consists of an ordinary differential equation with respect to the time variable. For a discussion of such second homogenization procedures we have to refer to the literature cited at the end of the introduction. Closely connected to the problems studied in this article is [52], where a second homogenization procedure for a phase transformation problem is presented.

4 Materials with temporally invariant microstructure

4.1 The microscopic and the homogenized initial-boundary value problems

In the remainder of this paper we study the initial-boundary value problem describing a material with a microstructure, which is temporally fixed. As in the case of the evolving microstructure the history functional in the homogenized problem is defined by an initial-boundary value problem in the representative volume element. In the case of fixed microstructure it is particularly suggestive to interpret this homogenized problem as a quasi-static problem for an inelastic material with a constitutive equation, which is an ordinary differential equation in an infinite dimensional Banach space.

Existence proofs for initial-boundary value problems to inelastic materials are often based on the idea to show that under suitable assumptions for the constitutive equations the initial-boundary value problem can be written as an evolution equation to a monotone operator. In [2] it is shown that even if the given constitutive equations do not satisfy these assumptions, they can sometimes be brought into a transformed form, in which the assumptions are fulfilled. Existence of solutions is then obtained from the general theory of such evolution equations if in a second step it can be shown that the operator is maximal monotone. This program has been carried out completely in [2] for some dynamic initial-boundary value problems, whereas for quasi-static problems only the reduction to an evolution equation to a monotone operator is given there.

The goal of this section is to show that under the same assumptions for the constitutive equations, which allow to reduce the initial-boundary value problem for an inelastic material with fixed microstructure to a monotone evolution equation also the homogenized problem with constitutive equation in an infinite dimensional Banach space can be reduced to a monotone evolution equation. The reduction to an evolution equation is carried out in section 4.2, the proof of monotonicity is given in section 4.3. Monotonicity is not enough to prove existence of solutions of the evolution equation. In addition it must be shown that the monotone operator is maximal and that the resulting family of monotone operators satisfies some regularity conditions. We must leave the determination of conditions for the constitutive equations assuring these properties and thus guaranteeing existence of solutions for the homogenized problem to later investigations. Also, the problem, to show that solutions of the microscopic problem tend to solutions of the homogenized problem if the scale of the microstructure goes to zero, is left open in this work.

We begin with the formulation of the microscopic and the homogenized initial-boundary value problems. We assume that the elasticity tensor D is a periodic function of the space variable x, but is independent of the time variable t. Moreover, we assume that the misfit strain ε^* is negligible. In this case the order parameter S is not needed to describe the microstructure. Therefore we obtain the mathematical model for a material with temporally fixed microstructure from the initial-boundary value problem (3.1)–(3.8) by droping the relations (3.4)–(3.6) and omiting the term ε^* in (3.2).

Thus, let $\Omega \subseteq \mathbb{R}^3$ be a bounded open set with smooth boundary. For every $y \in \mathbb{R}^3$ let $D(y) : \mathcal{S}^3 \to \mathcal{S}^3$ be a linear mapping, which is symmetric and positive definite. Let $f : \mathbb{R}^3 \times \hat{\Delta}(f) \to \mathbb{R}^N$ be a given map with $\hat{\Delta}(f) \subseteq \mathcal{S}^3 \times \mathbb{R}^N$. We assume that $y \mapsto D(y)$ and $y \mapsto f(y, T, z)$ are sufficiently smooth periodic functions with periodicity cell $Y \subseteq \mathbb{R}^3$. The periodicity cell is assumed to satisfy (3.10). Let $\eta > 0$ be a parameter, $B : \mathbb{R}^N \to \mathcal{S}^3$ be a linear mapping and $z^{(0)} : \Omega \to \mathbb{R}^N$ be given initial data. The microscopic initial-boundary value problem is

$$
\begin{aligned}
-\operatorname{div}_x T(x,t) &= b(x,t) && (4.1)\\
T(x,t) &= D(\frac{x}{\eta})(\varepsilon(\nabla_x u(x,t)) - Bz(x,t)) && (4.2)\\
z_t(x,t) &= f(\frac{x}{\eta},\, T(x,t),\, z(x,t))\,, && (4.3)\\
T(x,t)n(x) &= 0, \quad x \in \partial\Omega, \quad t \geq 0 && (4.4)\\
z(x,0) &= z^{(0)}(x), \quad x \in \Omega. && (4.5)
\end{aligned}
$$

To study the homogenization of this system we consider initial data of the form

$$
z^{(0)}(x) = z_0^{(0)}(x, \frac{x}{\eta}), \quad x \in \Omega, \tag{4.6}
$$

with a sufficiently regular function $z_0^{(0)} : \Omega \times \mathbb{R}^3 \to \mathbb{R}^N$. It is assumed that for every $x \in \Omega$ the function $y \mapsto z_0^{(0)}(x, y)$ is periodic with periodicity cell Y. For such initial data the analysis of Section 3.2 can be repeated. The resulting homogenized system is essentially equal to (3.36)–(3.38). To state the homogenized initial-boundary value problem precisely, let the mean value operator M_Y and the space $\mathcal{D}_0$ be defined as in Section 3.2. A scalar product on $L^2(Y)$ is defined by

$$
[v, w] = \int_Y (D(y)^{-1} v(y)) : w(y)\, dy.
$$

By $P : L^2(Y) \to \mathcal{D}_0 \subseteq L^2(Y)$ we denote the projector onto $\mathcal{D}_0$, which is orthogonal with respect to the scalar product $[v, w]$.

Definition 4.1 *The homogenized initial-boundary value problem associated to the problem* (4.1)–(4.6) *is given by*

$$
\begin{aligned}
-\operatorname{div}_x T_\infty(x,t) &= b(x,t), && (4.7)\\
T_\infty(x,t) &= \mathcal{F}_{s\le t}(\nabla_x u_0(x,s),x), && (4.8)\\
T_\infty(x,t)n(x) &= 0, \quad x\in\partial\Omega, \quad t\ge 0. && (4.9)
\end{aligned}
$$

Here the history functional $\nabla_x u_0(x,\cdot) \mapsto T_\infty(x,\cdot) = \mathcal{F}_{s\le t}(\nabla_x u_0(x,s),x)$ *is defined by the equation*

$$T_\infty(x,t) = M_Y T_0(x,\cdot,t), \tag{4.10}$$

which yields the mean stress T_∞ as a function of the micro stress T_0, and by the initial-boundary value problem, which defines T_0 and which consists of the equations

$$
\begin{aligned}
T_0(x,\cdot,t) &= P\{D(\cdot)(\varepsilon(\nabla_x u_0(x,t)) - Bz_0(x,\cdot,t))\}, && (4.11)\\
\frac{\partial}{\partial t} z_0(x,y,t) &= f(y, T_0(x,y,t), z_0(x,y,t)), && (4.12)
\end{aligned}
$$

and of the boundary and initial conditions

$$y \mapsto (T_0(x,y,t), z_0(x,y,t)) \textit{ is periodic with periodicity cell } Y, \tag{4.13}$$

$$z_0(x,y,0) = z_0^{(0)}(x,y), \quad (x,y)\in\Omega\times\mathbb{R}^3. \tag{4.14}$$

Remark. The periodicity requirement for T_0 in (4.13) can be dropped, since it is implied by the definition of the projection P.

From this formulation of the homogenized problem we see that it is a quasi-static problem for an inelastic material, whose history functional $\mathcal{F}_{s\le t}$ is defined by the system (4.11), (4.12) of ordinary differential equations in an infinite dimensional Banach space. Depending on the properties of f, the solution $(y,t)\mapsto z_0(x,y,t)$ of this differential equation can for every fixed t lie in the Banach space of functions on $\mathbb{R}^3$ periodic with periodicity cell Y and contained in $L^p(Y)$ for a suitable p, or it can lie in a Banach space of measures.

Just as in the homogenized problem to the evolving microstructure, we can also take another point of view and replace the equation (4.11) by the equivalent pair of equations

$$
\begin{aligned}
\operatorname{div}_y T_0(x,y,t) &= 0,\\
T_0(x,y,t) &= D(y)(\varepsilon(\nabla_x u_0(x,t) + \nabla_y u_1(x,y,t)) - Bz_0(x,y,t)),
\end{aligned}
$$

which must be supplemented by the periodicity condition

$$y \mapsto (u_1(x,y,t), T_0(x,y,t)) \text{ is periodic with periodicity cell } Y.$$

For every $x \in \Omega$, the equations (4.12)–(4.14) together with this pair of equations and with the periodicity condition constitute an initial-boundary value problem for the unknown function $(y,t) \mapsto (u_1, T_0, z_0)(x,y,t)$ in the domain $Y \times \mathbb{R}^+$, which has the same form as the problem (4.1)–(4.5). The function u_1 is the micro deformation.

For all these considerations we refer to the scholia after Definition 3.11.

4.2 Reduction of the homogenized system to an evolution equation

In this section we reduce the homogenized initial-boundary value problem to an evolution equation. The reduction follows in all essential details the reduction of quasi-static initial-boundary value problems to inelastic materials given in Section 3.2 of [2]. However, in the more complicated case of the homogenized problem properties of several linear spaces and linear operators play a role, which must first be determined. Before we carry out the reduction, we first collect the information needed about these spaces and operators in several lemmas:

We assume that the symmetric linear mapping $D(y) : \mathcal{S}^3 \to \mathcal{S}^3$ is uniformly positive definite: There exists a constant $c > 0$ with

$$(D(y)F) : F \geq c|F|^2$$

for all $y \in \mathbb{R}^3$ and all $F \in \mathcal{S}^3$. The bounded linear operator $\mathcal{P} : \mathcal{D}_0 \to \mathcal{D}_0$ is defined by

$$\mathcal{P}v = P(D(\cdot)v(\cdot)), \quad v \in \mathcal{D}_0 .$$

Lemma 4.2 *The operator $\mathcal{P}$ is selfadjoint with respect to the scalar product*

$$(v,w) = \int_Y v(y) : w(y)\, dy$$

on $\mathcal{D}_0$ and positive definite.

Proof: $D(y)$ is symmetric and positive definite, hence $D(y)^{-1}$ exists and is symmetric. By definition the projection P is orthogonal with respect to the scalar product $[v,w]$ on $L^2(Y)$. Hence P is selfadjoint. For $v, w \in \mathcal{D}_0$ we thus obtain

$$(\mathcal{P}v, w) \;=\; \int_Y [P(D(\cdot)v(\cdot))](y) : w(y)\, dy$$

$$
\begin{aligned}
&= \int_Y D(y)^{-1}[P(D(\cdot)v(\cdot))](y) : D(y)w(y)\,dy \\
&= \int_Y D(y)^{-1}[P(D(\cdot)v(\cdot))](y) : [P(D(\cdot)w(\cdot))](y)\,dy \\
&= \int_Y D(y)^{-1}D(y)v(y) : [P(D(\cdot)w(\cdot))](y)\,dy \\
&= \int_Y v(y) : [P(D(\cdot)w(\cdot))](y)\,dy = (v, \mathcal{P}w).
\end{aligned}
$$

Therefore $\mathcal{P}$ is selfadjoint. To see that $\mathcal{P}$ is positive definite, note that the above calculation also yields

$$
(\mathcal{P}v, v) = \int_Y D(y)^{-1}[P(D(\cdot)v(\cdot))](y) : [P(D(\cdot)v(\cdot))](y)\,dy = [\mathcal{P}v, \mathcal{P}v] \geq 0\,.
$$

It follows that $\mathcal{P}$ is positive definite if $\mathcal{P}v = P(D(\cdot)v(\cdot)) \neq 0$ for all $v \in \mathcal{D}_0$ with $v \neq 0$, hence if $\ker \mathcal{P} = \{0\}$. Now, if $v \in \ker \mathcal{P}$, then $D(\cdot)v(\cdot) \in \ker P = \mathcal{D}_0^{\perp}$. Since $v \in \mathcal{D}_0$, this implies

$$
0 = [v, D(\cdot)v(\cdot)] = \int_Y (D^{-1}(y)v(y)) : D(y)v(y)\,dy = \int_Y v(y) : v(y)\,dy,
$$

whence $v = 0$. This proves that $\mathcal{P}$ is positive definite. The proof is complete.

Next we need to collect some information about the kernel of the operator $\operatorname{div}_x M_Y$. First we define precisely how we want to understand this operator.

Definition 4.3 *The domain of definition of* $\operatorname{div}_x M_Y$ *consists of all functions* $w \in L^2(\Omega \times Y, \mathcal{S}^3)$, *for which* $v \in L^2(\Omega, \mathbb{R}^3)$ *exists satisfying*

$$
-\int_\Omega (M_Y w(x,\cdot)) : \nabla_x \varphi(x)\,dx = \int_\Omega v(x) \cdot \varphi(x)\,dx,
$$

for all $\varphi \in H_1(\Omega, \mathbb{R}^3)$. *Obviously,* v *is uniquely defined by this equation. We thus define*

$$
(\operatorname{div}_x M_Y)w = v.
$$

Clearly, this means that the domain of definition of $\operatorname{div}_x M_Y$ consists of all w, for which div_x can be applied to $x \mapsto (M_Y w(x,\cdot))$ in the weak sense, and which in the weak sense satisfy

$$
[M_Y w(x,\cdot)]n(x) = 0, \quad x \in \partial\Omega.
$$

By $\mathcal{K}$ we denote the kernel of the operator $\operatorname{div}_x M_Y$. Then $\mathcal{K}$ is the subspace of all functions $w \in L^2(\Omega \times Y, \mathcal{S}^3)$ with

$$
\int_\Omega (M_Y w(x,\cdot)) : \nabla_x \varphi(x)\,dx = 0 \tag{4.15}
$$

for all $\varphi \in H_1(\Omega, \mathbb{R}^3)$. The subspace $\mathcal{K}$ is closed. The orthogonal space of $\mathcal{K}$ in $L^2(\Omega \times Y, \mathcal{S}^3)$ with respect to the scalar product

$$(v, w)_{\Omega\times Y} = \int_\Omega \int_Y v(x,y) : w(x,y)\, dxdy$$

is denoted by $\mathcal{K}^\perp$.

Lemma 4.4 (i) *The space $\mathcal{K}$ consists of all functions w of the form*

$$w(x,y) = w_0(x) + w_1(x,y), \tag{4.16}$$

where $w_0 \in L^2(\Omega, \mathcal{S}^3)$ satisfies

$$\operatorname{div}_x w_0 = 0, \quad w_0(x)n(x) = 0, \quad x \in \partial\Omega \tag{4.17}$$

in the weak sense, and where $w_1 \in L^2(\Omega \times Y, \mathcal{S}^3)$ satisfies

$$M_Y w_1(x, \cdot) = 0, \quad x \in \Omega. \tag{4.18}$$

(ii) *We have*

$$\mathcal{K}^\perp = \{(x,y) \mapsto \varepsilon(\nabla_x v(x)) \mid v \in H_1(\Omega, \mathbb{R}^3)\}. \tag{4.19}$$

Remark. w_0 satisfies (4.17) in the weak sense if $\int_\Omega w_0(x) : \nabla\varphi(x)\, dx = 0$ for all $\varphi \in H_1(\Omega, \mathbb{R}^3)$, of course. (ii) means that all functions of the set $\mathcal{K}^\perp$ are constant with respect to the y-variable.

Proof: (i) Assume that $w = w_0 + w_1$ with $w_0,\ w_1$ satisfying (4.17), (4.18). For $\varphi \in H_1(\Omega, \mathbb{R}^3)$ we then have because of (3.10)

$$\begin{aligned}
\int_\Omega (M_Y w(x,\cdot)) : \nabla_x \varphi(x)\, dx &= \int_\Omega (M_Y w_0(x) + M_Y w_1(x,\cdot)) : \nabla_x \varphi(x)\, dx \\
&= \int_\Omega w_0(x) : \nabla_x \varphi(x)\, dx = 0,
\end{aligned}$$

whence $w \in \mathcal{K}$. On the other hand, assume that $w \in \mathcal{K}$. We set $w_0(x) = M_Y w(x,\cdot)$ and $w_1 = w - w_0$. Then $w(x,y) = w_0(x) + w_1(x,y)$ and w_1 satisfies (4.18), since

$$\begin{aligned}
&M_Y w_1(x,\cdot) = M_Y w(x,\cdot) - M_Y w_0(x) \\
&= M_Y w(x,\cdot) - w_0(x) = M_Y w(x,\cdot) - M_Y w(x,\cdot) = 0,
\end{aligned}$$

where we used (3.10) again. Moreover, w_0 satisfies (4.17), since for $\varphi \in H_1(\Omega, \mathbb{R}^3)$

$$\int_\Omega w_0(x) : \nabla_x \varphi(x)\, dx = \int_\Omega \int_Y w_0(x)\, dy : \nabla_x \varphi(x)\, dx$$

$$= \int_\Omega (M_Y w_0(x) + M_Y w_1(x,\cdot)) : \nabla_x \varphi(x)\, dx$$

$$= \int_\Omega (M_Y w(x,\cdot)) : \nabla_x \varphi(x)\, dx = 0.$$

This proves (i).
(ii) Let $M_Y^T : L^2(\Omega, \mathcal{S}^3) \to L^2(\Omega \times Y, \mathcal{S}^3)$ denote the transpose operator of $M_Y : L^2(\Omega \times Y, \mathcal{S}^3) \to L^2(\Omega, \mathcal{S}^3)$. It is immediately seen that

$$(M_Y^T v)(x,y) = v(x)$$

for all $v \in L^2(\Omega, \mathcal{S}^3)$ and all $(x,y) \in \Omega \times Y$.

Since $M_Y w(x,\cdot)$ is a symmetric matrix for all $w \in L^2(\Omega \times Y, \mathcal{S}^3)$, it follows that

$$(M_Y w(x,\cdot)) : \nabla_x \varphi(x) = (M_Y w(x,\cdot)) : \varepsilon(\nabla_x \varphi(x)).$$

Therefore, by (4.15), $\mathcal{K}$ is the set of all $w \in L^2(\Omega \times Y, \mathcal{S}^3)$ with

$$\begin{aligned} 0 &= \int_\Omega (M_Y w(x,\cdot)) : \nabla_x \varphi(x)\, dx \\ &= \int_\Omega (M_Y w(x,\cdot)) : \varepsilon(\nabla_x \varphi(x))\, dx \\ &= \int_\Omega \int_Y w(x,y) : [M_Y^T(\varepsilon(\nabla_x \varphi))](x,y)\, dy dx, \end{aligned}$$

for all $\varphi \in H_1(\Omega, \mathbb{R}^3)$. Thus, $\mathcal{K}$ is the orthogonal space of the subspace

$$\{M_Y^T(\varepsilon(\nabla_x \varphi)) \mid \varphi \in H_1(\Omega, \mathbb{R}^3)\} = \{(x,y) \mapsto \varepsilon(\nabla_x \varphi(x)) \mid \varphi \in H_1(\Omega, \mathbb{R}^3)\}.$$

Since this subspace is closed, it is equal to $\mathcal{K}^\perp$. This proves (ii).

Because $\mathcal{K}$ is a closed subspace of $L^2(\Omega \times Y, \mathcal{S}^3)$, we can define the orthogonal projection $\Pi_1 : L^2(\Omega \times Y, \mathcal{S}^3) \to \mathcal{K} \subseteq L^2(\Omega \times Y, \mathcal{S}^3)$ onto $\mathcal{K}$. Orthogonality is meant with respect to the scalar product $(v,w)_{\Omega \times Y}$. By $\Pi_2 = I - \Pi_1$ we denote the orthogonal projection to the orthogonal space $\mathcal{K}^\perp$ of $\mathcal{K}$.

An operator defined on a subspace of $L^2(\Omega \times Y, \mathcal{S}^3)$ can be introduced using the operator $\mathcal{P} : \mathcal{D}_0 \to \mathcal{D}_0$ as follows: Since this operator is linear, bounded, selfadjoint and positive definite, it defines by

$$((x,y) \mapsto v(x,y)) \mapsto ((x,y) \mapsto (\mathcal{P} v(x,\cdot))(y)) \tag{4.20}$$

a bounded linear operator on

$$L^2(\Omega, \mathcal{D}_0) = \{v \in L^2(\Omega \times Y, \mathcal{S}^3) \mid v(x, \cdot) \in \mathcal{D}_0 \text{ for almost all } x\},$$

which is also selfadjoint with respect to the scalar product $(v, w)_{\Omega \times Y}$ and positive definite, and which we denote by the same symbol $\mathcal{P} : L^2(\Omega, \mathcal{D}_0) \to L^2(\Omega, \mathcal{D}_0)$. Of course, the same considerations apply to the inverse $\mathcal{P}^{-1} : L^2(\Omega, \mathcal{D}_0) \to L^2(\Omega, \mathcal{D}_0)$.

The next lemma contains information about these operators:

Lemma 4.5 (i) *We have*

$$\Pi_1(L^2(\Omega, \mathcal{D}_0)) \subseteq \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0), \quad \Pi_2(L^2(\Omega \times Y, \mathcal{S}^3)) \subseteq L^2(\Omega, \mathcal{D}_0)$$

(ii) *The operator $\Pi_1 \mathcal{P}^{-1}$ maps the subspace $\mathcal{K} \cap L^2(\Omega, \mathcal{D}_0)$ of $L^2(\Omega \times Y, \mathcal{S}^3)$ into itself, and*

$$\Pi_1 \mathcal{P}^{-1} : \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0) \to \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0)$$

is selfadjoint and positive definite.

Proof: (i) Lemma 4.4 (ii) implies for the range $R(\Pi_2)$ of the projection Π_2 that

$$R(\Pi_2) = \mathcal{K}^\perp = \{(x, y) \mapsto \varepsilon(\nabla_x v(x)) \mid v \in H_1(\Omega, \mathbb{R}^3)\} \subseteq L^2(\Omega, \mathcal{D}_0),$$

since functions $w(x, y) = \varepsilon(\nabla_x v(x))$ are periodic with respect to y and satisfy $\operatorname{div}_y v(x, y) = 0$. For $v \in L^2(\Omega, \mathcal{D}_0)$ we thus have

$$\Pi_1 v = (I - \Pi_2) v = v - \Pi_2 v \in L^2(\Omega, \mathcal{D}_0),$$

hence $\Pi_1(L^2(\Omega, \mathcal{D}_0)) \subseteq \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0)$. The proof of (i) is complete.
(ii) Since $\mathcal{P}^{-1} : L^2(\Omega, \mathcal{D}_0) \to L^2(\Omega, \mathcal{D}_0)$ we conclude from (i) that

$$\Pi_1 \mathcal{P}^{-1} : \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0) \to \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0).$$

To see that this operator is selfadjoint and positive definite, let $v,\ w \in \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0)$. Then $\Pi_1 v = v$ and $\Pi_1 w = w$. Since the orthogonal projection Π_1 is selfadjoint on $L^2(\Omega \times Y)$ and $\mathcal{P}^{-1}$ is selfadjoint on $L^2(\Omega, \mathcal{D}_0)$, we thus obtain

$$\begin{aligned}(\Pi_1 \mathcal{P}^{-1} v, w)_{\Omega \times Y} &= (\mathcal{P}^{-1} v, \Pi_1 w)_{\Omega \times Y} = (\mathcal{P}^{-1} v, w)_{\Omega \times Y} \\ &= (v, \mathcal{P}^{-1} w)_{\Omega \times Y} = (\Pi_1 v, \mathcal{P}^{-1} w)_{\Omega \times Y} = (v, \Pi_1 \mathcal{P}^{-1} w)_{\Omega \times Y}\,.\end{aligned}$$

This shows that $\Pi_1 \mathcal{P}^{-1}$ is selfadjoint. From this computation it also follows that for $v \neq 0$

$$(\Pi_1 \mathcal{P}^{-1} v, v)_{\Omega \times Y} = (\mathcal{P}^{-1} v, v)_{\Omega \times Y} > 0,$$

since $\mathcal{P}^{-1}$ is positive definite on $L^2(\Omega, \mathcal{D}_0)$. Consequently, $\Pi_1 \mathcal{P}^{-1}$ is positive definite. This proves the lemma.

Reduction to an evolution equation. With these lemmas we can reduce the homogenized initial-boundary value problem to an evolution equation. We use the following notation: For functions v and w defined on $\Omega \times \mathbb{R}^+$ and on $\Omega \times Y \times \mathbb{R}^+$, respectively, which take values in some space V, we denote by $v(t)$ and $w(t)$ the functions

$$x \mapsto v(x,t) : \Omega \to V \text{ and } (x,y) \mapsto w(x,y,t) : \Omega \times Y \to V,$$

respectively.

Since by Lemma 4.2 the operator $\mathcal{P} : \mathcal{D}_0 \to \mathcal{D}_0$ is selfadjoint and positive definite, it has a selfadjoint and positive definite inverse $\mathcal{P}^{-1} : \mathcal{D}_0 \to \mathcal{D}_0$. Because P is the projection to $\mathcal{D}_0$, the terms on both sides of the equation (4.11) belong to the domain of definition of $\mathcal{P}^{-1}$. Therefore we can apply $\mathcal{P}^{-1}$ to this equation and obtain together with (4.7) and (4.10)

$$-\operatorname{div}_x \left(M_Y T_0(x,\cdot,t) \right) = b(x,t) \tag{4.21}$$

$$\mathcal{P}^{-1} T_0(x,\cdot,t) = \varepsilon(\nabla_x u_0(x,t)) - \mathcal{P}^{-1} P(D(\cdot) B z_0(x,\cdot,t)). \tag{4.22}$$

Here we used that $\varepsilon(\nabla_x u_0(x,t))$ can be considered to be a function of (x,y,t), which is constant with respect to y. Since constant functions belong to $\mathcal{D}_0$, we have $\varepsilon(\nabla_x u_0(x,t)) \in \mathcal{D}_0$ for all (x,t), which yields

$$\mathcal{P}^{-1} P(D(\cdot)\varepsilon(\nabla_x u_0(x,t))) = \mathcal{P}^{-1}\mathcal{P}\varepsilon(\nabla_x u_0(x,t)) = \varepsilon(\nabla_x u_0(x,t)).$$

In the second term on the right of (4.22) this simplification is not possible, since $B z_0(x,\cdot,t) \notin \mathcal{D}_0$, in general. Hence this function does not belong to the domain of definition of $\mathcal{P}$.

In the next step we insert $T_0 = \Pi_1 T_0 + \Pi_2 T_0$ into (4.21). Because Π_1 projects to the kernel of the operator $\operatorname{div}_x M_Y$, we obtain

$$\begin{aligned} -\operatorname{div}_x M_Y T_0(t) &= -\operatorname{div}_x M_Y(\Pi_1 T_0)(t) - \operatorname{div}_x M_Y(\Pi_2 T_0)(t) \\ &= -\operatorname{div}_x M_Y(\Pi_2 T_0)(t) = b(t). \end{aligned} \tag{4.23}$$

Here we used that $T_0(t)$ and, as a consequence, also $\Pi_2 T_0(t)$ belong to the domain of definition of $\operatorname{div}_x M_Y$. This is guaranteed by the boundary condition (4.9). We continue by applying Π_1 to (4.22), which results in

$$\begin{aligned} \Pi_1 \mathcal{P}^{-1} T_0(t) &= \Pi_1 \varepsilon(\nabla_x u_0(t)) - \Pi_1 \mathcal{P}^{-1} P(DBz_0(t)) \\ &= -\Pi_1 \mathcal{P}^{-1} P(DBz_0(t)), \end{aligned}$$

since (4.19) implies $\varepsilon(\nabla_x u_0(t)) \in \mathcal{K}^\perp$ and since $\mathcal{K}^\perp = \ker \Pi_1$. Using $T_0(t) \in L^2(\Omega, \mathcal{D}_0)$, we conclude from Lemma 4.5 (i) that $\Pi_1 T_0(t)$, $\Pi_2 T_0(t) \in L^2(\Omega, \mathcal{D}_0)$, whence $\Pi_1 T_0(t)$ and $\Pi_2 T_0(t)$ both belong to the domain of definition of $\mathcal{P}^{-1}$. Consequently, $\mathcal{P}^{-1}T_0(t) = \mathcal{P}^{-1}\Pi_1 T_0(t) + \mathcal{P}^{-1}\Pi_2 T_0(t)$, which shows that the last equation can be written in the form

$$\Pi_1\mathcal{P}^{-1}(\Pi_1 T_0)(t) = -\Pi_1\mathcal{P}^{-1}P(DBz_0(t)) - \Pi_1\mathcal{P}^{-1}(\Pi_2 T_0)(t). \tag{4.24}$$

Because the mapping

$$\Pi_1\mathcal{P}^{-1} : \mathcal{K}\cap L^2(\Omega,\mathcal{D}_0) \to \mathcal{K}\cap L^2(\Omega,\mathcal{D}_0)$$

is selfadjoint and positive definite, it has an inverse, which is also selfadjoint and positive definite. We denote this inverse by $(\Pi_1\mathcal{P}^{-1})^{-1}$. Because the three functions $T_0(t)$, $\mathcal{P}^{-1}P(DBz_0(t))$ and $\mathcal{P}^{-1}(\Pi_2 T_0)(t)$ all are contained in $L^2(\Omega,\mathcal{D}_0)$, we can invoke Lemma 4.5 (i) again to conclude from this fact that $\Pi_1 T_0(t)$ and both terms on the right hand side of (4.24) belong to the subspace $\mathcal{K}\cap L^2(\Omega,\mathcal{D}_0)$, the domain of definition of $(\Pi_1\mathcal{P}^{-1})^{-1}$. Therefore we can apply this inverse to all terms of the equation (4.24). Differentiation of the resulting equation and insertion of (4.12) for $\frac{\partial}{\partial t}z_0$ yields

$$\begin{aligned}\frac{\partial}{\partial t}(\Pi_1 T_0)(\cdot,\cdot\cdot,t) &= -(\Pi_1\mathcal{P}^{-1})^{-1}\Pi_1\mathcal{P}^{-1}P(D(\cdot\cdot)Bf(\cdot\cdot,T_0(\cdot,\cdot\cdot,t),z_0(\cdot,\cdot\cdot,t)))\\ &\quad - (\Pi_1\mathcal{P}^{-1})^{-1}\Pi_1\mathcal{P}^{-1}\frac{\partial}{\partial t}(\Pi_2 T_0)(\cdot,\cdot\cdot,t).\end{aligned} \tag{4.25}$$

We note that in this equation $(\Pi_1\mathcal{P}^{-1})^{-1}\Pi_1\mathcal{P}^{-1}$ can not be replaced by the identity, since $(\Pi_1\mathcal{P}^{-1})^{-1}$ is the inverse of $\Pi_1\mathcal{P}^{-1}$ on $\mathcal{K}\cap L^2(\Omega,\mathcal{D}_0)$. However, $P(DBf) \notin \mathcal{K}\cap L^2(\Omega,\mathcal{D}_0)$ and $(\Pi_2 T_0)_t \notin \mathcal{K}\cap L^2(\Omega,\mathcal{D}_0)$, in general.

If we replace T_0 by $\Pi_1 T_0 + \Pi_2 T_0$ in the argument of f, then we obtain from (4.25) the evolution equation for $\Pi_1 T_0$ which we sought. We state this evolution equation and the equation (4.23) for $\Pi_2 T_0$ in the following

Theorem 4.6 *Assume that (u_0, T_0, z_0) is a function which has the properties*

$$u_0(t) \in H_1(\Omega,\mathbb{R}^3) \tag{4.26}$$

$$T_0(t),\ \frac{\partial}{\partial t}T_0(t) \in L^2(\Omega\times Y,\mathcal{S}^3) \tag{4.27}$$

$$z_0(t),\ \frac{\partial}{\partial t}z_0(t) \in L^2(\Omega\times Y,\mathcal{S}^3), \tag{4.28}$$

for almost all $t\in\mathbb{R}^+$, and which satisfies the homogenized initial-boundary value problem (4.7)–(4.14). Then T_0 and z_0 satisfy on $\Omega\times Y\times R^+$ the equations

$$-\mathrm{div}_x\, M_Y(\Pi_2 T_0) = b(x,t) \tag{4.29}$$

$$\begin{aligned}\frac{\partial}{\partial t}(\Pi_1 T_0) &= -(\Pi_1\mathcal{P}^{-1})^{-1}\Pi_1\mathcal{P}^{-1}P(D(\cdot)Bf(\cdot,\Pi_1 T_0+\Pi_2 T_0,z_0))\\ &\quad - (\Pi_1\mathcal{P}^{-1})^{-1}\Pi_1\mathcal{P}^{-1}(\Pi_2 T_0)_t\end{aligned} \tag{4.30}$$

$$\frac{\partial}{\partial t}z_0 = f(\cdot,\Pi_1 T_0+\Pi_2 T_0,z_0), \tag{4.31}$$

on $\partial\Omega \times \mathbb{R}^+$ the boundary condition

$$[M_Y \Pi_2 T_0(x,\cdot,t)]n(x) = 0, \tag{4.32}$$

and on $\Omega \times Y$ the initial conditions

$$\begin{aligned}(\Pi_1 T_0)(x,\cdot,0) &= -(\Pi_1\mathcal{P}^{-1})^{-1}\Pi_1\mathcal{P}^{-1}P(D(\cdot)Bz_0^{(0)}(x,\cdot)) \\ &\qquad - (\Pi_1\mathcal{P}^{-1})^{-1}\Pi_1\mathcal{P}^{-1}(\Pi_2 T_0)(x,\cdot,0) \qquad (4.33)\\ z_0(x,y,0) &= z_0^{(0)}(x,y). \qquad (4.34)\end{aligned}$$

Conversely, if T_0 and z_0 are periodic with respect to y, fulfill (4.27)*,* (4.28) *and satisfy* (4.29)–(4.34)*, then a unique function u_0 exists satisfying* (4.26)*, such that the function (u_0, T_0, z_0) solves the homogenized initial-boundary value problem* (4.7)–(4.14).

Scholium. Before we give the remaining parts of the proof of this theorem, we interpret the equations (4.29)–(4.34). The equations (4.29) and (4.32) belong together and are meant in the weak sense. Together they mean that for almost all t the function $(x,y) \mapsto (\Pi_2 T_0)(x,y,t)$ must belong to the domain of definition of the operator $\operatorname{div}_x M_Y$ introduced in Definition 4.3 and that the application of this operator to $\Pi_2 T_0$ yields $x \mapsto b(x,t)$. Since by definition Π_2 maps to the orthogonal space of the kernel of $\operatorname{div}_x M_Y$, the function $\Pi_2 T_0$ is uniquely determined by (4.29) and (4.32). Hence, if these two equations can be solved for almost all t, then the component $\Pi_2 T_0$ of T_0 in the space $\mathcal{K}^\perp$ is known. Thus, the unknowns in (4.30), (4.31) and (4.33), (4.34) are z_0 and the component $\Pi_1 T_0$ of T_0 in the space $\mathcal{K}$. Therefore, (4.30), (4.31) is a system of evolution equations for the functions $\Pi_1 T_0$ and z_0 to the initial conditions (4.33), (4.34). If this system can be solved, then $T_0 = \Pi_1 T_0 + \Pi_2 T_0$ and z_0 are known. By the statement of the theorem, u_0 can be determined such that (u_0, T_0, z_0) satisfy the homogenized initial-boundary value problem.

Proof: We already proved that (4.29), (4.30) follow from (4.7), (4.11). The equations (4.31) and (4.34) coincide with (4.12) and (4.14). With $T_\infty(x,t) = M_Y T_0(x,\cdot,t)$, the boundary condition (4.9) can be written in the form

$$(M_Y T_0(x,\cdot,t))n(x) = 0, \quad (x,t) \in \partial\Omega \times \mathbb{R}^+.$$

The boundary condition (4.32) follows from this equation and from

$$\Pi_2 T_0 = T_0 - \Pi_1 T_0\,,$$

since by definition Π_1 is the projection to the kernel of the operator $\operatorname{div}_x M_Y$; the function $\Pi_1 T_0$ thus satisfies

$$[M_Y \Pi_1 T_0(x,\cdot,t)]n(x) = 0$$

on $\partial\Omega \times \mathbb{R}^+$ in the weak sense. Finally, the initial condition (4.33) for $\Pi_1 T_0$ is obtained by application of the operator $(\Pi_1 \mathcal{P}^{-1})^{-1}$ to (4.24) and insertion of the initial data for z_0 in the resulting equation.

Conversely, assume that (4.29)–(4.34) are satisfied. We use (4.31) to replace f in (4.30) by $\frac{\partial}{\partial t} z_0$ and integrate the resulting equation with respect to t. Insertion of the initial condition (4.33) for $\Pi_1 T_0$ and application of the operator $\Pi_1 \mathcal{P}^{-1}$ to the resulting equation yields (4.24), which can be written in the form

$$\Pi_1 \mathcal{P}^{-1} T_0 = -\Pi_1 \mathcal{P}^{-1} P(D(\cdot) B z_0).$$

Since $\ker \Pi_1 = \mathcal{K}^\perp$, this equation and Lemma 4.4 (ii) imply that for almost every t there exists a function $(x \mapsto u_0(x,t)) \in H_1(\Omega, \mathbb{R}^3)$ such that (4.22) is satisfied. Moreover, (4.21) follows directly from (4.29). From (4.21), (4.22) we obtain (4.7) and (4.11) by application of $\mathcal{P}$ to (4.22). The equations (4.12), (4.14) and (4.9) result directly from (4.31), (4.34) and (4.32). This proves the theorem.

Remark. The hypothesis $z_0(t)$, $\frac{\partial}{\partial t} z_0(t) \in L^2(\Omega \times Y, \mathcal{S}^3)$ in Theorem 4.6 is questionable. In fact, from the theory of quasi-static problems it is known that $z_0(t)$ belongs to L^2 only if f satisfies growth restrictions, which are not satisfied in most constitutive models derived in the engineering sciences. In general, z_0 belongs to L^p or to a space of measures, depending on the properties of f. However, we believe that the preceding reasoning can be modified to hold also in situations where z_0 belongs to these more general spaces.

4.3 Monotonicity of the evolution equation

The crucial difficulty in proving that the homogenized initial-boundary value problem has a solution is to show that the evolution system (4.30) and (4.31) is solvable. Here we prove that if f is a monotone vector field, then this evolution system can be written as an evolution equation of the form

$$\tau_t(t) = -A(t)\tau(t) + g(t) \tag{4.35}$$

with a known function g and with a family $\{A(t)\}_{t\geq 0}$ of monotone operators. This is an essential step in proving existence of solutions for the homogenized system. Of course, monotonicity of $A(t)$ alone is not sufficient for existence of solutions of (4.35). It is necessary that $A(t)$ is maximal monotone and that the family $\{A(t)\}_{t\geq 0}$ satisfies additional regularity conditions, cf. [16, 23]. Whether these additional conditions are satisfied is an open question, not only for the homogenized system, but also for the original system, where a similar, but simpler reduction to an evolution equation is possible.

In order to keep the discussion simple, we restrict ourselves in the following investigations to constitutive equations (4.3) of the form

$$z_t = f(\frac{x}{\eta}, T),$$

where the function f does not depend on the internal variables z explicitly. Many simple constitutive equations used in the engineering sciences are of this form, cf. [2]. We remark however, that the following considerations go through for considerably more general functions f, which also depend on the internal variables z explicitly.

So, assume that

$$f = f(y, T).$$

In this case (4.29), (4.30) and the boundary condition (4.32) form a closed system for $\Pi_1 T_0$ and $\Pi_2 T_0$, and the evolution equation (4.31) for the internal variables z_0 can be dropped. To simplify the notation we set

$$\tau = \Pi_1 T_0\,, \quad \sigma = \Pi_2 T_0\,.$$

Then $\tau = \tau(x, y, t)$, $\sigma = \sigma(x, y, t)$ and $\tau(t) \in \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0)$, $\sigma(t) \in \mathcal{K}^\perp$ for almost every $t \geq 0$. The equation (4.30) takes the form

$$\tau_t(t) = -(\Pi_1 \mathcal{P}^{-1})^{-1} \Pi_1 \mathcal{P}^{-1} P(D(\cdot) B f(\cdot, \tau(t) + \sigma(t))) - (\Pi_1 \mathcal{P}^{-1})^{-1} \Pi_1 \mathcal{P}^{-1} \sigma_t(t)\,. \tag{4.36}$$

According to the discussion following Theorem 4.6, the function $\sigma(t)$ is uniquely determined by (4.29) and (4.32). Therefore σ and the function $g = (\Pi_1 \mathcal{P}^{-1})^{-1} \Pi_1 \mathcal{P}^{-1} \sigma_t$ can be considered to be known. With this function g the equation (4.36) can thus be written in the form (4.35), if we define the operator $A(t) = A(\sigma(t))$ by

$$A(\sigma(t))\hat{\tau} = (\Pi_1 \mathcal{P}^{-1})^{-1} \Pi_1 \mathcal{P}^{-1} P(D(\cdot) B f(\cdot, \hat{\tau} + \sigma(t))), \tag{4.37}$$

for every $\hat{\tau}$ from the domain of definition $\Delta(\sigma(t))$ of $A(\sigma(t))$. For $\Delta(\sigma(t))$ we choose the set of all functions $\hat{\tau} \in \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0)$, for which

$$((x, y) \mapsto f(y, \hat{\tau}(x, y) + \sigma(x, y, t))) \in L^2(\Omega \times Y, \mathbb{R}^N) \tag{4.38}$$

holds. With this choice we have

$$A(\sigma(t)) : \Delta(\sigma(t)) \subseteq \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0) \to \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0).$$

To see this, note that by definition of the projection P, the relation (4.38) implies

$$x \mapsto P(D(\cdot) B f(\cdot, \hat{\tau}(x, \cdot) + \sigma(x, \cdot, t))) \in L^2(\Omega, \mathcal{D}_0).$$

Since $\mathcal{P}^{-1} : L^2(\Omega, \mathcal{D}_0) \to L^2(\Omega, \mathcal{D}_0)$, we thus obtain from Lemma 4.5 (i) that for $\hat{\tau} \in \Delta(\sigma(t))$

$$\Pi_1 \mathcal{P}^{-1} P(D(\cdot) B f(\cdot, \hat{\tau} + \sigma(t))) \in \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0),$$

which together with Lemma 4.5 (ii) and with the definition of $A(\sigma(t))$ yields

$$A(\sigma(t))\hat{\tau} \in \mathcal{K} \cap L^2(\Omega, \mathcal{D}_0).$$

This proves the assertion. In passing we note that, as indicated in the notation, the operator $A(t) = A(\sigma(t))$ depends on the time t only via the known function $\sigma(t)$.

A mapping $A : \Delta(A) \subseteq H \to H$ on a Hilbert space H with the scalar product (v, w) is monotone if

$$(Av - Aw, v - w) \geq 0$$

for all $v, w \in \Delta(A)$. Here $\Delta(A)$ denotes the domain of A. We shall prove that $A(\sigma(t))$ is a monotone operator on $\mathcal{K} \cap L^2(\Omega, \mathcal{D}_0)$ for almost all t, if this Hilbert space is equipped with the scalar product defined as follows: In Lemma 4.5 it was proved that $\Pi_1 \mathcal{P}^{-1}$ is selfadjoint and positive definite on the Hilbert space $\mathcal{K} \cap L^2(\Omega, \mathcal{D}_0)$ with the scalar product $(v, w)_{\Omega \times Y} = \int_\Omega \int_Y v(x, y) : w(x, y)\, dydx$. Using this, we define the new scalar product on $\mathcal{K} \cap L^2(\Omega, \mathcal{D}_0)$ by

$$\langle v, w \rangle = \int_\Omega \int_Y (\Pi_1 \mathcal{P}^{-1} v) : w \, dydx\,. \tag{4.39}$$

Theorem 4.7 *Let $f : \mathbb{R}^3 \times \mathcal{S}^3 \to \mathbb{R}^N$ be a given function and $B : \mathbb{R}^N \to \mathcal{S}^3$ be a linear mapping. Assume that for every $y \in \mathbb{R}^3$ the vector field $\tilde{\tau} \mapsto Bf(y, \tilde{\tau}) : \mathcal{S}^3 \to \mathcal{S}^3$ is monotone:*

$$(Bf(y, \tilde{\tau}_1) - Bf(y, \tilde{\tau}_2)) : (\tilde{\tau}_1 - \tilde{\tau}_2) \geq 0, \tag{4.40}$$

for all $\tilde{\tau}_1,\ \tilde{\tau}_2 \in \mathcal{S}^3$. Then for every $\sigma \in \mathcal{K}^\perp \subseteq L^2(\Omega \times Y, \mathcal{S}^3)$ the operator $A(\sigma)$ defined in (4.37) *is monotone on $\mathcal{K} \cap L^2(\Omega, \mathcal{D}_0)$, if this space is equipped with the scalar product $\langle v, w \rangle$.*

Proof: Let $\tau_1,\ \tau_2 \in \Delta(\sigma)$. Then (4.37) and (4.39) yield

$$\begin{aligned}
&\langle A(\sigma)\tau_1 - A(\sigma)\tau_2,\, \tau_1 - \tau_2 \rangle \\
&= \int\limits_{\Omega \times Y} \Big(\Pi_1 \mathcal{P}^{-1} [PD(\cdot)Bf(\cdot, \tau_1 + \sigma) - PD(\cdot)Bf(\cdot, \tau_2 + \sigma)] \Big) : (\tau_1 - \tau_2) d(x, y) \\
&= \int\limits_{\Omega \times Y} \Big(\Pi_1 \mathcal{P}^{-1} PD(\cdot)(Bf(\cdot, \tau_1 + \sigma) - Bf(\cdot, \tau_2 + \sigma)) \Big) : (\tau_1 - \tau_2)\, d(x, y) =: J_1,
\end{aligned}$$

where we used the linearity of $\Pi_1 \mathcal{P}^{-1}$ and of P. Since $\Pi_1 : L^2(\Omega \times Y, \mathcal{S}^3) \to \mathcal{K} \subseteq L^2(\Omega \times Y, \mathcal{S}^3)$ is orthogonal with respect to the scalar product $(v, w)_{\Omega \times Y}$

and since $\tau_1 - \tau_2 \in \mathcal{K}$, hence $\Pi_1(\tau_1 - \tau_2) = \tau_1 - \tau_2$, we obtain that

$$\begin{aligned}
J_1 &= \int_\Omega \int_Y \Big(\mathcal{P}^{-1} P(D(\cdot)(Bf(\cdot,\tau_1+\sigma) - Bf(\cdot,\tau_2+\sigma)))\Big) : (\tau_1 - \tau_2)\, dydx \\
&= \int_\Omega \int_Y \Big(P(D(\cdot)(Bf(\cdot,\tau_1+\sigma) - Bf(\cdot,\tau_2+\sigma)))\Big) : \mathcal{P}^{-1}(\tau_1 - \tau_2)\, dydx \\
&=: J_2\,.
\end{aligned}$$

Here we used that $\mathcal{P}$ defined in (4.20) and also $\mathcal{P}^{-1}$ are selfadjoint on $L^2(\Omega,\mathcal{D}_0)$ with respect to the scalar product $(v,w)_{\Omega\times Y}$. Note that P projects to $\mathcal{D}_0$, hence $PD(\cdot)(Bf(\cdot,\tau_1+\sigma) - Bf(\cdot,\tau_2+\sigma)) \in L^2(\Omega,\mathcal{D}_0)$ and $\tau_1 - \tau_2 \in L^2(\Omega,\mathcal{D}_0)$. We next use that $P : L^2(Y) \to \mathcal{D}_0 \subseteq L^2(Y)$ is orthogonal with respect to the scalar product $[v,w] = \int_Y (D(y)^{-1}v(y)) : w(y)\, dy$. For all $v,\ w \in L^2(Y)$ we thus have

$$\begin{aligned}
&\int_Y [P(Dv)] : w\, dy = \int_Y [D(y)^{-1} P(D(\cdot)v(\cdot))] : D(y)w(y)\, dy \\
&= \int_Y D(y)^{-1} D(y) v(y) : P(D(\cdot)w(\cdot))\, dy = \int_Y v : [P(Dw)]\, dy\,.
\end{aligned}$$

Using this relation, we obtain

$$\begin{aligned}
J_2 &= \int_\Omega \int_Y \Big(Bf(y,\tau_1+\sigma) - Bf(y,\tau_2+\sigma)\Big) : P(D(\cdot)\mathcal{P}^{-1}(\tau_1 - \tau_2))\, dydx \\
&= \int_\Omega \int_Y (Bf(y,\tau_1+\sigma) - Bf(y,\tau_2+\sigma)) : (\tau_1 - \tau_2)\, dydx \\
&= \int_\Omega \int_Y \Big[(Bf(y,(\tau_1+\sigma)(x,y)) - Bf(y,(\tau_2+\sigma)(x,y))\Big] \\
&\qquad\qquad : \Big[(\tau_1+\sigma)(x,y) - (\tau_2+\sigma)(x,y)\Big]\, dydx \\
&\geq 0.
\end{aligned}$$

The last inequality sign follows from the assumption (4.40). In this step we used that for $v \in L^2(\Omega,\mathcal{D}_0)$

$$P(D(\cdot)v(x,\cdot))(y) = (\mathcal{P}v)(x,y),$$

by definition of $\mathcal{P}$, hence $P(D(\cdot)\mathcal{P}^{-1}(\tau_1 - \tau_2)) = \mathcal{P}\mathcal{P}^{-1}(\tau_1 - \tau_2) = \tau_1 - \tau_2$.

This computation proves that the operator $A(\sigma)$ is monotone. The proof is complete.

Conclusion. The contributions of this article to the mathematical theory of phase transformations and to the homogenization of mathematical models from solid mechanics can be summarized as follows:

In Section 2 we derived a new mathematical model for the evolution in time of phase transitions. In this model the order parameter belongs to the space BV^{loc} of functions of bounded variation. Its evolution in time is rate dependent and is governed by a first order partial differential equation, a Hamilton-Jacobi equation. This model could be an alternative to the Cahn-Allen model.

Since the order parameter is of bounded variation, to determine the effective equations to this model it was necessary in Section 3 to study homogenization in the space BV^{loc}. This made it necessary to introduce the idea of a family of solutions of the microscopic initial-boundary value problem depending on the fast variable.

In Section 4 we reduced the homogenized system of partial differential equations for temporally invariant microstructure to an evolution equation. The reduction procedure generalizes the reduction given in [2] for the equations modeling inelastic solids. As a first step in the direction of an existence proof we showed that the resulting evolution equation is monotone.

It remains open whether the model suggested in Section 2 has a solution and whether the solution is unique. Moreover, it would be important to investigate this model numerically. Also,the proof of monotonicity in Section 4 should be extended to an existence proof for the homogenized system to temporally invariant microstructure. Subsequently, this homogenized system should be justified by proving that the solutions of the homogenized problem tend asymptotically to the solutions of the microscopic problem. In the last step, the same program should be carried out for the homogenized problem to evolving microstructure. Of these tasks, the existence proof for the homogenized system to invariant microstructure and the justification of this system seem to be the most accessible ones.

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