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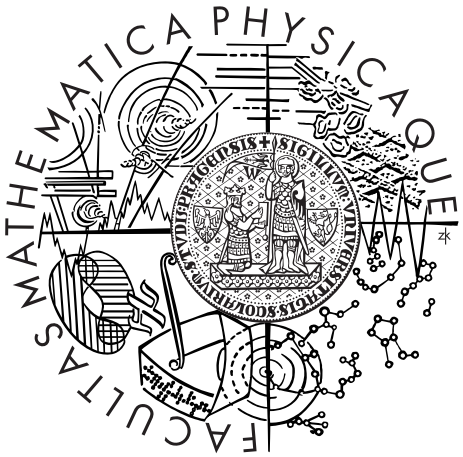

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Mathematical and computational modeling of shape-memory alloys

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I declare that I carried out this doctoral thesis independently, and only with the cited sources, literature and other professional sources.

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In Prague, June 22, 2012 Barbora Benešová

Název práce: Matematické a počítačové modelování materiálů s tvarovou pamětí
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Abstrakt: Tato dizertační práce se zabývá vývojem mesoskopického modelu monokrystalu slitin s pamětí tvaru zahrnujícího termodynamicky konsistentní popis termomechanických vazeb. Pod pojmem "mesoskopický" v tomto kontextu rozumíme schopnost modelu zachytit jemné prostorové oscilace deformačního gradientu pomocí gradientních Youngových měr. Existence řešení navrženého modelu byla dokázaná v tzv. "phase-field"-aproximaci pomocí přechodu z mikroskopického modelu obsahujícího člen popisující povrchovou energii. Tento přechod z fyzikálně relevantního modelu na jiné škále zajistí oprávněnost mesoskopické relaxace. Existence řešení byla také dokázána zpětnou Eulerovou časovou diskretizací. Tato metoda tvoří koncept numerického algoritmu, na němž byla založena počítačová implementace navrženého modelu. Ta byla dále optimalizována pro rychlostně nezávislý isotermální případ. Vybrané výsledky simulací spočítaných touto implementací jsou rovněž prezentovány. V neposlední řadě jsou uvedena zjemnění analýzy v případě konvexní obálky Helmholtzovy volné energie a odpovídající limita phase-field aproximace.

Klíčová slova: Martenzitická transformace, Relaxace, Youngovy míry, Termodynamika, Škálový přechod, Globální optimalizace v proměnných prostředích.

Title: Mathematical and computational modeling of shape-memory alloys
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Abstract: This dissertation thesis is concerned with developing a mesoscopic model for single crystalline shape-memory alloys including thermo-dynamically consistent thermo-mechanical coupling – here the term "mesoscopic" refers to the ability of the model to capture fine spatial oscillations of the deformation gradient by means of gradient Young measures. Existence of solutions to the devised model is proved in a "phase-field-like approach" by a scale transition from a microscopic model that features a term related to the interfacial energy; this scale transition from a physically relevant model justifies the mesoscopic relaxation. Further, existence of solutions is also proved by backward-Euler time discretization which forms a conceptual numerical algorithm. Based on this conceptual algorithm a computer implementation of the model has been developed and further optimized in the rate-independent isothermal setting; some calculations using this implementation are also presented. Finally, refinements s of the analysis in the convex case as well as a limit of the phase-field-like approach in this case are exposed, too.
Keywords: Martensitic transformation, Relaxation, Young measures, Thermodynamics, Scale transition, Global optimization in changing environments.

Contents

Preface: motivation, overview of main results

Motivation

Shape memory alloys (SMAs) are so-called *intelligent* (or *smart* or also *active*) materials that exhibit remarkable *hysteretic* stress/strain/temperature responses and, hence, are advantageous for a lot of applications in engineering and human medicine. In particular, SMAs have the ability to recover their original shape after deformation just by heat supply; this is referred to as the *shape-memory effect*.

The outstanding properties of SMAs are due to a diffusionless solid-to-solid *phase transformation*, called the *martensitic transition*; this transformation can be (and usually is) accompanied by fast spatial oscillations of the deformation gradient referred to as *microstructure*. It is exactly the *formation of microstructure* that play a *key role* in the behavior of SMAs because the material can compensate stress by a *reorientation* of the microstructure.

Mathematical and computational modeling of SMAs is challenging mainly because of their *multiscale character*, when changes in the crystalline structure have crucial impact on the macroscale. It has received huge attention during past three decades, cf. the monographs (Bhattacharya, 2003; Dolzmann, 2003; Frémond, 2002; Frémond and Miyazaki, 1996; Pitteri and Zanzotto, 2003). The variety of models is very large, ranging from atomistic to continuum mechanical, from the ones focusing on special loading regimes and/or particular phenomena to very general ones; cf. also (Roubíček, 2004) for a survey.

In order to model behavior of *single-crystalline* shape-memory alloys the so-called *mesoscopic* scale is advantageous since laboratory-sized specimen can be taken into account on this scale; models on this scale are based on relaxation in variational calculus using *gradient Young measures*. So far, on the mesoscopic scale, the following types of models have been scrutinized:

- Static models based on minimization of the Helmholtz free energy; cf. e.g. (Ball and James, 1987, 1992; Müller, 1999).

- Evolutionary isothermal variants of mesoscopic models prescribing a Helmholtz free energy and a dissipation potential; see (Kružík et al., 2005; Mielke and Roubíček, 2003).

- Evolutionary variants with a uniform temperature distribution in the specimen with temperature prescribed as a load; see (Mielke et al., 2009; Mielke and Petrov, 2007).

However, a mesoscopic model including *thermo-coupling effects* has been still missing although this coupling effects are *absolutely essential* for a complete description of

SMAs; in particular they play a key role when understanding the *shape-memory effect*.[1]

Aims

Since accurate models including thermomechanic coupling on the mesoscopic scale have still been missing a challenge the community working in this area faces can be summarized as:

Design a thermodynamically and mathematically consistent modeling framework for single crystalline SMAs on the mesoscopic scale that couples mechanic and thermal effects and gives instructions on numerical analysis. Furthermore, find an experiment-justified form of the constitutive parts of the modeling framework and implement the concrete model to be able to compare its predictions to experiments.

Within this thesis we contribute to this challenge, in particular the following goals have been set:

- To design a thermodynamically consistent modeling framework for single crystalline SMAs on the mesoscopic scale that couples mechanic and thermal effects but possibly posses restriction on the involved energy/dissipation representation.
- To prove existence of solutions to the system of equations/inclusions representing the modeling framework in a appropriate weak setting.
- To design a mathematically consistent discretization of system of equations/inclusions representing the modeling framework.
- To implement a simple model falling within the modeling framework and compare the results to theoretical predictions.

Overview of main results

The main results of this thesis and some of the papers developed within the work on it (namely (Benešová, 2009; Benešová, Kružík and Roubíček, 2012; Benešová and Roubíček, 2012; Benešová, 2011*a*,*b*)) contribute to all of the set goals, in particular results fall within the so-called "Modeling part" that is concerned with designing a modeling framework, within the "Analytical part" where existence of solutions is proved and the "Numerical part" on implementation; naturally there is a synergy between the respective parts. Although all three parts are treated, emphasis was laid upon the *analytical part*.

Modeling part

The modeling, we work within the framework of generalized standard materials in continuum mechanics (Chapter 3) and the *large strain setting*; let us sketch here the main modeling ideas and the effects that can be captured.

We fix $\Omega \subset \mathbb{R}^d$ as the reference configuration of the body, we define the *deformation* of the body $y : \Omega \to \mathbb{R}^d$ and a variable capturing the microstructure $\nu \in \mathscr{G}^p(\Omega; \mathbb{R}^{d\times d})$

[1] Such models exist on the macroscopic scale (e.g. (Frémond, 2002)); however, those models are mathematically much easier to handle, so we can borrow only very few ideas on mathematics from them.

being a *gradient Young measure*[2]. The set of state variables further includes the *temperature* $\theta : \Omega \to \mathbb{R}$ and, as an internal variable, a vectorial *phase-field* $\lambda : \Omega \to \mathbb{R}^{M+1}$. This phase-field corresponds (up to a possible small mismatch) to *the volume fraction* of the high-temperature phases or to one of the so-called *variants* in the low-temperature phase in some material point of the SMA specimen; its evolution is, in the presented modeling approach, related with energy dissipation during phase transformation.

Within the framework of generalized standard solids (cf. (Halphen and Nguyen, 1975)), we constitutively define two potentials: the Gibbs free energy $\mathcal{G} = \mathcal{G}(t, y, \nu, \lambda, \theta)$ and a dissipation potential $R = R(\dot{\lambda})$, a careful choice of these potentials will allow us to capture qualitatively some of the important phenomena in SMAs. The Gibbs free energy is proposed in the form (see (5.6))

$$\mathcal{G}(t, y, \nu, \lambda, \theta) = \underbrace{\int_\Omega \widetilde{\psi}_0(\cdot, \lambda, \theta) \bullet \nu \, \mathrm{d}x}_{\text{stored energy}} + \underbrace{\mathcal{Q}_\varkappa(\lambda - L \bullet \nu)}_{\text{mismatch term}} - \underbrace{\int_\Omega f(t, \cdot) \cdot y \, \mathrm{d}x - \int_{\Gamma_\mathrm{N}} g(t, \cdot) \cdot y \, \mathrm{d}S}_{\text{energy of the applied load}},$$

where, " $\bullet$ " is the *"momentum" operator* (cf. the Nomenclature), $f(t, x)$ is the applied volume force and $g(t, x)$ the applied surface force on one part of the boundary denoted Γ_N (cf. the Nomenclature). In the penalty-like mismatch term we use a quadratic form $\mathcal{Q}_\varkappa : L^2(\Omega) \to \mathbb{R}$, defined through (5.2), we assume that $\varkappa$ is large causing only a presumably small mismatch between λ and $L \bullet \nu$, the latter being the volume fraction stemming from microstructure.

The specific *free energy* $\widetilde{\psi}_0(F, \lambda, \theta)$ is assumed in the following, partly linear form (see (5.1))

$$\widetilde{\psi}_0(F, \lambda, \theta) = \underbrace{\phi_0(\theta)}_{\substack{\text{thermal} \\ \text{part}}} + \underbrace{\phi_1(F)}_{\substack{\text{multiwell} \\ \text{mechanical part}}} + \underbrace{(\theta - \theta_\mathrm{tr})\vec{a} \cdot \lambda}_{\substack{\text{thermomechanical} \\ \text{coupling}}},$$

where θ_tr is the transformation temperature (see Chapter 1) and $\vec{a}$ is related to the transformation entropy (see Section 5.1); the linear thermomechanic coupling is the leading term in the chemical energy and ϕ_1 has typically a *multiwell structure* chosen e.g. like in (Ball and James, 1987; Kružík et al., 2005).

Due to the structure of ϕ_1, the model predicts *formation of microstructure* in the specimen, cf. (Ball and James, 1987; Bhattacharya, 2003; Müller, 1999); thermomechanic coupling term on the other hand drives the *shape-memory effect*. Thus, not only the shape-memory effect but heating/cooling accompanying evolution of microstructure can be captured.

It is well known and documented by many experiments (cf. e.g. (Novák et al., 2008; Otsuka and Ren, 2005)) that the martensitic transformation is a dissipative process. Hence, the dissipation potential $R(\dot{\lambda})$ is proposed to be of the form (see (5.9))

$$R(\dot{\lambda}) = \int_\Omega \rho_q(\dot{\lambda}) \, \mathrm{d}x,$$

with ρ_q of order $q \geq 2$ but non-smooth at $\dot{\lambda} = 0$ to model the martensitic transformation as an activated process. However, since the dissipation potential depends only on $\dot{\lambda}$, purely geometric changes of the microstructure that do not change ratio of the phases[3] are, on this scale, considered non-dissipative.

[2] See Chapter 2 for details on gradient Young measures.

[3] For simplification, we use in this introduction the term "phases", but also changes of the ratio of variants are considered dissipative.

The evolution of the system is the, following (3.17)-(3.18), governed by the following Biot's type system of inclusions (note that we assume quasi-static evolution)

$$\partial_\nu\big(\mathcal{G}(t,y,\nu,\lambda,\theta)+\delta_{\mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^{d\times d})}\big)\ni 0, \tag{1}$$

$$\partial_{\dot\lambda}R(\dot\lambda)+\partial_\lambda\mathcal{G}(t,y,\nu,\lambda,\theta)\ni 0, \tag{2}$$

with (due to the non-convexity of the set $\mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^{d\times d})$) rather formally understood (sub-)differentials ∂ and $\delta_{\mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^d)}$ the indicator function to the set $\mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^d)$. The system is completed by intial/boundary conditions and a *heat equation* for θ. This equation will be derived from the local balance of the *entropy* $s=-[\widetilde{\psi}_0]'_\theta$ that reads (cf. (3.19))

$$\theta\dot s+\operatorname{div} j = \text{ heat-production rate} = \partial\rho_q(\dot\lambda)\cdot\dot\lambda, \tag{3}$$

where j stands for the heat flux which assumed to be governed by the *Fourier law* $j=-\mathbb{K}\nabla\theta$ with the *heat-conductivity* tensor $\mathbb{K}=\mathbb{K}(\lambda,\theta)$.

Note that, due to the mentioned Gibbs relation $s=-[\widetilde{\psi}_0(\nabla y,\lambda,\theta)]'_\theta(\lambda,\theta)=-\phi_0'(\theta)-\lambda$, the model also predicts heating of parts of the specimen that undergo austenite-to-martensite transformation and cooling in the parts undergoing the reverse transformation, as actually observed during experiments.

Let us stress that, contrary to (Mielke and Petrov, 2007), within our approach *the shape-memory effect* can be modeled when prescribing the temperature only at the boundary and *not* in the whole specimen. Also, when designing the model, special attention was paid to thermodynamic consistency; cf. Section 5.2.

Analytical part

As far as mathematical analysis is concerned, we devise the following weak formulation of the problem the system (1)-(3) in Section 5.3, namely in Definition 5.4 and are able to prove the following theorem:

Theorem 0.1. *Let (A1)-(A7)*[4] *hold. Then at least one weak solution* (y,ν,λ,w) *to the problem* (1)-(3) *in accord with Definition 5.4 does exist.*

In other words, we can prove existence of solutions to (1)-(3) formulated weakly.

Two different methods have been devised to prove Theorem 0.1, each one of them of its own *particular* importance. One method relies on finding a related modeling framework that, however, *takes the interfacial energy into account* and is thus suitable *only for microscopical grains/specimen* – we would call this framework "microscopic" – and passing to the limit if the interfacial energy becomes negligible. This method is particularly important *from the modeling point of view* since in surpasses scales and, thus, *justifies* the mesoscopic approach based on relaxation. The other method relies on *time-discretization* and, thus, gives *instructions on numerical analysis*.

The method of approximation through approximation by microscopic models is exposed in Section 5.4 and has been published in (Benešová and Roubíček, 2012) while the method based on time-discretization is contained in Section 5.5; this result is published for the first time in this thesis. Let us, in this short overview, point out the basic ingredients of both methods of proof.

[4] Assumptions (A1)-(A7) are stated in Section 5.3.

The related microscopic framework, we need to prove Theorem 0.1, is obtained by setting, within the framework of generalized standard solids, the Gibbs free energy to

$$\mathcal{G}_\varepsilon(t,y,\lambda,\theta) = \underbrace{\int_\Omega \widetilde{\psi}_0(F,\lambda,\theta)\,\mathrm{d}x}_{\text{stored energy}} + \underbrace{\int_\Omega \frac{\varepsilon}{2}|\nabla^2 y|^2\,\mathrm{d}x}_{\text{interfacial energy}} + \underbrace{\mathcal{Q}_\varkappa(\lambda - L(\nabla y))}_{\text{mismatch term}} \\ \underbrace{- \int_\Omega f(t,\cdot)\cdot y\,\mathrm{d}x - \int_{\Gamma_{\mathrm{N}}} g(t,\cdot)\cdot y\,\mathrm{d}S}_{\text{energy of the applied load}}.$$

Here, the stored energy, the applied loads as well as the mismatch term are taken from the mesoscopic model and, as announced, an interfacial energy is added. Note that in this case we work *only* with the deformation y – because of the interfacial energy there is no need for relaxations. Physically this corresponds to the fact, that these models are fitted to smaller scales at which the oscillations of the deformation gradient can be resolved *fully* and not just in an average sense.

Furthermore, we set the dissipation potential to

$$R_\varepsilon(\dot{y},\dot{\lambda}) = \int_\Omega \rho_q(\dot{\lambda}) + \varepsilon|\nabla\dot{y}|\,\mathrm{d}x,$$

where the first term is corresponds to the mesoscopic model while the second term counts a small activation energy to vary the deformation gradient and can be conceptually related to the concept of wiggly energies as proposed in (Abeyaratne et al., 1996; James, 1996).

The proof in Section 5.4 is then based on passing to the limit $\varepsilon \to 0$.

As far as time-discretization is concerned, we employ the Rothe method; i.e., we introduce an equi-distant partition $0 = t_0 \le t_1 \le \ldots \le t_N = T$ with τ the distance between the partition points and call $(y_\tau^k, \nu_\tau^k, \lambda_\tau^k, \theta_\tau^k)$ the time-discrete weak solutions to the presented model, if they satisfy:

The **minimization problem for** λ with given λ_τ^{k-1}, θ_τ^{k-1}, y_τ^{k-1} and ν_τ^{k-1}:

$$\left.\begin{array}{ll} \text{Minimize} & \mathcal{G}(t_k, y_\tau^{k-1}, \nu_\tau^{k-1}, \lambda, \theta_\tau^{k-1}) + \tau R\left(\frac{\lambda-\lambda_\tau^{k-1}}{\tau}\right) + \tau\int_\Omega |\lambda|^{2q} \\ \text{subject to} & \lambda \in L^{2q}(\Omega;\mathbb{R}^{M+1}). \end{array}\right\} \tag{4}$$

The **minimization problem for** (y,ν) with given λ_τ^k, θ_τ^{k-1}, y_τ^{k-1} :

$$\left.\begin{array}{ll} \text{Minimize} & \mathcal{G}(t_k, y, \nu, \lambda_\tau^k, \theta_\tau^{k-1}) \\ \text{subject to} & (y,\nu) \in W^{1,p}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^d) \times \mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d}), \end{array}\right\} \tag{5}$$

and the discretized heat equation.

The devised discretization relies on a kind of "altering minimization" of the increment of the Gibbs free energy plus dissipation – a time discretization based on minimization of this quantity is well known in the isothermal, rate-independent setting (Francfort and Mielke, 2006; Mielke and Theil, 2004). The proof in Section 5.5 is the based on passing to the limit $\tau \to 0$.

Besides these two methods of proof, we present in Chapter 6 changes in the mathematical treatment in the *convex* case; in particular we prove an existence proof based on yet on the more common discretization based on minimization of the increment of the Gibbs free energy plus dissipation – this result has been obtained in (Benešová, Kružík and Roubíček, 2012). Moreover, we are able to pass to the limit $\varkappa \to \infty$, i.e., in this case, we show that models containing the "mismatch term" approach those for which the constrain $\lambda = L\bullet\nu$ is fulfilled. This *justifies* the penalty-like "mismatch term" in the non-convex case – this result is published for the first time within this thesis.

Numerical part

Within this thesis, a numerical implementation of the system of equations/inclusions (1)-(3) has been based on the proposed time-discretization; details are given in Chapter 7. Within computation the hardest part is to compute the *global minima* of the Gibbs free energy in a very large state space having, possibly, several thousands degrees of freedom. To this end, we tested several minimization algorithms and adapted them to our case. Moreover, in the isothermal, rate-independent case further optimalizations based on necessary conditions have been obtained. While the results on the isothermal, rate-independent case have already been published in (Benešová, 2011*a*), simulations on thermally coupled case are, for the first time, published here.

Results beyond the main scope of the thesis

Within the preparation of this thesis also two results were obtained that are beyond the main scope of the topic of the resulting thesis but still connected to the area of modeling of SMAs. Namely, the following two results were obtained:

- In (Benešová, Kružík and Pathó, 2012) a subclass of gradient Young measures, namely those that are (roughly) generated by sequences of gradients in $\mathbb{R}^{d\times d}$ bounded together with their inverse, has been obtained. This result represents a contribution to an important, still open, problem on how to design relaxed energies to those that enforce the local non-interpenetration condition. The problem is also related to mesoscopic models of SMAs that are based on relaxation and, since the problem is still open, the interpenetration condition has to be omitted. We present a summary of the results in Section 2.3.2.

- In (Sedlák et al., 2012) a macroscopic model for the SMA $NiTi$ has been devised. The model can be applied for complex loading situations, captures anisotropy and the effect of the so-called R-phase. The results from this paper are not a part of the thesis.

Overview of all papers prepared within the work on this thesis

- In (Benešová, 2009) calculations within a rate-indepentent model for the R-phase of $NiTi$ were presented.

- In (Benešová, 2011*a*) enhancements of the global-optimum search in the rate-independent setting were proposed; cf. Section 7.2.

- In (Benešová, 2011*b*) the thermally coupled model presented in this thesis has been introduced; cf. Chapter 5.

- In (Benešová, Kružík and Roubíček, 2012) a thermally coupled model for micromagnetics has been studied; for the main mathematical outcomes see Chapter 6.

- In (Benešová and Roubíček, 2012) the micro-to-meso scale transition in the thermally coupled case has been investigated; cf. Section 5.4.

- In (Benešová, Kružík and Pathó, 2012) a subclass of Young measures relevant to problems in elasticity has been characterized; cf. Section 2.3.2.

- In (Sedlák et al., 2012) a macroscopic model for SMAs has been proposed.

Nomenclature

M	number of martensitic variants
d	dimension of the problem
θ_{tr}	transformation temperature; cf. Section 1.1
Ω	an open bounded domain in $\mathbb{R}^d$ with Lipschitz boundary; the reference configuration except for Chapter 2
$[0,T]$	a time-interval on which the evolutionary problems are set
Γ	the boundary of the domain Ω
Γ_{D}	the part of the boundary of the domain Ω where Dirichlet boundary conditions are considered
Γ_{N}	the part of the boundary of the domain Ω where Neumann boundary conditions are considered
Q	$= [0,T] \times \Omega$
Σ	$= [0,T] \times \Gamma$
Σ_{D}	$= [0,T] \times \Gamma_{\mathrm{D}}$
Σ_{N}	$= [0,T] \times \Gamma_{\mathrm{N}}$
C	a *generic* constant; possibly independent of some variables, if so it is explicitly stated
id	the identity mapping from $\mathbb{R}^{d\times d} \to \mathbb{R}^{d\times d}$
$\mathbb{I}$	the identity matrix in $\mathbb{R}^{d\times d}$
$\mathrm{O}(d)$	the set of orthogonal matrices in $\mathbb{R}^{d\times d}$
$\mathrm{SO}(d)$	the set of rotations in $\mathbb{R}^{d\times d}$
δ_S	the indicator function (in the sense of convex analysis) to the set S
$C(\Omega)$	the space of continuous functions on Ω equipped with the norm $\|u\| = \max_{x\in\bar{\Omega}} \|u(x)\|$
$C^k(\Omega)$	the space of functions that have continuous derivatives up to the order k on Ω
$C(\bar{\Omega};V)$	the space of continuous functions on $\bar{\Omega}$ with values in some Banach space V equipped with the norm $\|u\| = \max_{x\in\bar{\Omega}} \|u(x)\|_V$
$C([0,T];V)$	the space of continuous functions on $[0,T]$ with values in some Banach space V equipped with the norm $\|u\| = \max_{t\in[0,T]} \|u(t)\|_V$
$L^p(\Omega;V)$	the space of p-integrable functions on Ω with values in some Banach space V equipped with the norm (for $p \in [1,\infty)$) $\|u\| = \left(\int_\Omega \|u(x)\|_V^p \mathrm{d}x\right)^{1/p}$; if $V = \mathbb{R}$ we simply write $L^p(\Omega)$
$L^p([0,T];V)$	the space of p-integrable functions on $[0,T]$ with values in some Banach space V equipped with the norm (for $p \in [1,\infty)$)$\|u\| = \left(\int_0^T \|u(t)\|_V^p \mathrm{d}x\right)^{1/p}$; if $V = \mathbb{R}$ we simply write $L^p([0,T])$

$\mathcal{M}(\mathbb{R}^{d\times d})$	the space of Radon measures on $\mathbb{R}^{d\times d}$
$W^{1,p}(\Omega;V)$	the Sobolev space of p-integrable functions on Ω whose distributional derivatives are also p-integrable with values in a Banach space V equipped with the norm (for $p\in[1,\infty)$)$\|u\| = \left(\int_\Omega \|u(x)\|_V^p + \|\nabla u(x)\|_V^p \mathrm{d}x\right)^{1/p}$; if $V=\mathbb{R}$ we simply write $W^{1,p}(\Omega)$
$W^{1,p}([0,T];V)$	the Sobolev space of p-integrable functions on $[0,T]$ whose distributional derivatives are also p-integrable with values in a Banach space V equipped with the norm (for $p\in[1,\infty)$) $\|u\| = \left(\int_0^T \|u(t)\|_V^p + \|\nabla u(t)\|_V^p \mathrm{d}t\right)^{1/p}$; if $V=\mathbb{R}$ we simply write $W^{1,p}([0,T])$
$W^{1,p}_{\Gamma_{\mathrm{D}}}(\Omega;V)$	the space of Sobolev functions with $y(x)=x$ on $\Gamma_{\mathrm{D}}\subset\partial\Omega$
$W^{2,2}(\Omega;V)$	the Sobolev space of quadratically integrable functions on Ω whose first and second distributional derivatives are also quadratically integrable with values in a Banach space V equipped with the norm $\|u\| = \left(\int_\Omega \|u(x)\|_V^2 + \|\nabla u(x)\|_V^2 + \|\nabla^2 u(x)\|_V^2 \mathrm{d}x\right)^{1/2}$; if $V=\mathbb{R}$ we simply write $W^{2,2}(\Omega)$
$H^{-1}(\Omega;V)$	the dual space to $W_0^{1,2}(\Omega;V^*)$ with V^* the dual to the reflexive Banach space V.
$BV([0,T];V)$	the space of function with bounded variation with values in the Banach space V equipped with the norm $\|u\| = \sup\left\{\sum_{i=1}^N \|u(t_{i+1})-u(t_i)\|_V;\ \text{over all partitions } 0\le t_1\le t_2\ldots\le t_N\le T\right\}$
$B([0,T];V)$	the spaces of bounded *not necessarily measurable* functions on $[0,T]$ with values in the Banach space V
p'	the conjugate exponent to $p\in[1,\infty]$, namely $p'=\frac{p}{p-1}$
p^*	the exponent in the embedding $W^{1,p}(\Omega;V)\hookrightarrow L^{p^*}(\Omega;V)$, namely $p^*=\frac{dp}{d-p}$ if $\Omega\subset\mathbb{R}^d$ and $p<d$, p^* is anything in $[1,\infty)$ if $p=d$ and $p^*=\infty$ if $p>d$
$p^\sharp$	the exponent in the trace operator $u\to u_{\|\Gamma} : W^{1,p}(\Omega;V)\to L^{p^\sharp}(\Gamma;V)$, namely $p^\sharp=\frac{dp-p}{d-p}$ if $\Omega\subset\mathbb{R}^d$ and $p<d$, $p^\sharp$ is anything in $[1,\infty)$ if $p=d$ and $p^\sharp=\infty$ if $p>d$
$W^{\alpha,p}(\Omega;V)$	the Sobolev space of p-integrable functions on Ω having fractional derivatives (for $\alpha\in(0,1)$)
$\mathscr{Y}(\Omega;\mathbb{R}^{d\times d})$	the set of Young measures defined in (2.18)
$\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d})$	the set of L^p-Young measures defined in (2.19)
$\mathscr{G}(\Omega;\mathbb{R}^{d\times d})$	the set of gradient Young measures defined in (2.21)
$\mathscr{G}^p(\Omega;\mathbb{R}^{d\times d})$	the set of L^p gradient Young measures defined in (2.22)
$\mathscr{G}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d})$	the set of gradient Young measures generated by sequences being identity on Γ_{D} defined in (2.23)
$\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d})$	the set of L^p gradient Young measures generated by sequences being identity on Γ_{D} defined in (2.24)
$\bullet$	the momentum operator defined through (2.17)

Chapter 1

Introduction to shape-memory alloys

Shape-memory alloys (SMAs) belong to the class of so-called *smart* materials owing to their outstanding thermo-mechanic properties. Namely, the following characteristic responses to thermo-mechanical loading (cycles) are of particular interest to physicists, engineers as well as mathematicians (see e.g. the monographs and review papers (Bhattacharya, 2003; Dolzmann, 2003; Frémond, 2002; Otsuka and Ren, 2005; Pitteri and Zanzotto, 2003; Roubíček, 2004)): the *shape-memory effect*, *pseudo-plasticity* and *super-elasticity*.

The *shape-memory effect* refers to the possibility to induce mechanic deformation far beyond thermal expansion by heat supply. In more detail, whenever a SMA-specimen is deformed at a temperature lower than a critical temperature $\theta_{\rm tr}$ (will be defined in Section 1.1, below), it can recover its original shape if it is heated to temperature above $\theta_{\rm tr}$. The shape-memory effect was first observed in 1951 for an Au-Cd alloy and has been documented in many experimental papers for various alloys since then (cf. e.g. the review paper (Otsuka and Ren, 2005) and references therein).

Further, when a SMA-specimen is mechanically loaded at a temperature lower than $\theta_{\rm tr}$ it maintains its new shape, even after all loads are released. This is similar to a plastic response and hence this effect is referred to as *pseudo-plasticity*. Note, that the material can recover its original shape upon heating.

If kept at a temperature higher that $\theta_{\rm tr}$ a SMA-specimen can be mechanically loaded up to several percents and, when all loads are released, it returns to its original shape. This effect is know as *super-elasticity*.

Due to these unique responses to thermo-mechanical loads, SMAs have a strong potential to be applied in a variety of technical systems like self-erecting space antennae, helicopter blades, surgical tools, reinforcement for arteries and veins, self-locking rivets or actuators; in some of them SMAs are already used routinely today (Hartl et al., 2009; Machado and Savi, 2003).

Let us stress, at this point, that this work will consider only *single-crystalline* SMA specimen.

1.1 Martensitic transformation

All the remarkable temperature-stress-strain responses of SMAs are due to a *diffusionless*, *first-order* solid-to-solid phase transition, called the *martensitic transformation* a SMA can undergo when exposed to thermal or mechanic loads. This transformation is characterized by a change in the symmetry of the crystal lattice of the alloy. Namely, a stress-free SMA-specimen is at high temperatures (above $\theta_{\rm tr}$) stable in the *austenitic*

phase, characterized by a higher symmetry of the atomic lattice (usually cubic symmetry). At low temperatures in stress-free condition the stable phase, *martensite*, is characterized by lower symmetry of its atomic lattice. It is exactly this lower symmetry that allows the martensite to be found in several so-called *variants*, which can be combined to form *microstructure* (cf. Section 1.2). Changes in this microstructure are often called *martensite reorientation* and form a key ingredient for thermo-mechanical responses described above. In more detail this is explained in Section 1.2, making use of the description of the phases/variants of a SMA by deformation gradients.

It has been proven experimentally (cf. e.g. (Otsuka and Ren, 2005)) that the martensitic transformation is a *dissipative process*. So is martensite reorientation (Sedlák et al., 2012); an important experimental finding backing this claim is the so-called *martensite stabilization*. Namely, is has been observed, on single- as well as on polycrystals, that the temperature at which a SMA-specimen transforms from martensite back to austenite is considerably higher when it has been subject to (specific) mechanical loads before heating (Liu and Favier, 2000; Picornell et al., 2006).

For modelling, we shall follow, in this work, e.g (Bhattacharya, 2003) and assume that, in the static situation, there is *exactly one* temperature θ_{tr} at which austenite and martensite are energetically equivalent. Above this temperature, *only* austenite is (energetically) stable (in stress-free configuration), below it *only* martensite. This approach has also been exploited by a large number of other authors, e.g. (Aubry et al., 2003; Auricchio and Petrini, 2002; Ball and James, 1992; Kružík et al., 2005; Mielke and Roubíček, 2003; Sadjadpour and Bhattacharya, 2007*b*). We refer to this specific temperature as the *transformation temperature*; however, as explained below, this temperature does not, even in stress-free situations, need to be the one at which austenite *actually* transforms to martensite or vice versa.

In experiments, often a whole range of temperatures in which martensite and austenite co-exist in the specimen is observed (Liu and Favier, 2000; Otsuka and Ren, 2005; Šittner et al., 2004); moreover this range differs when the transformation proceeds from austenite to martensite from the one observed in the reverse transformation. Yet, this is rather evidence that the martensitic transformation is dissipative than a falsification of our assumption of one transformation temperature. Indeed, if the amount of energy that the material would lose in dissipation by performing a martensitic transformation in the whole specimen is larger that the energy gain by performing it, it might be advantageous to transform only partly. Similarly, martensite stabilization (Liu and Favier, 2000; Picornell et al., 2006) is rather an indication for the presence of dissipation due to martensite reorientation rather than falsifying our assumption.

Some experiments also hint to the idea that if the single-crystalline SMA specimen did not have corners at the martensitic transformation would not start upon heating (Ball et al., 2011). Still, we are entitled to use one transformation temperature, if we understand it to be, as already pointed out, the temperature of *energetic equilibrium between austenite and martensite*. Indeed, it has been shown in (Ball et al., 2011) that the experimentally observed phenomenon can be explained by the mechanic incompatibility of an austenitic nucleus in the martensite specimen apart from corners; i.e. if a nucleus apart the corner formed the specimen had to break within the simplified model used in (Ball et al., 2011).[1]

[1] In (Ball et al., 2011) the Helmholtz free energy was chosen to be finite only for deformations gradients corresponding to austenite/the variants of martensite and their rotations. However, since elastic constants of SMAs are rather large compared to other parameters entering mesoscopic models, a similar behavior can be expected within model presented in Chapters 4 and 5.

1.2 Crystalline structure and its relation to continuum mechanics

Since it is the crystalline structure that characterizes the different phases of a SMA, let us briefly review its description and how it can be translated in to continuum mechanics.

As any other solid crystalline material, SMAs consist of atoms that are arranged into a crystal lattices described by a set of three linearly independent vectors $\{e_a\}$. The set of points

$$L(e_a) = \{x \in \mathbb{R}^d, x = \sum_a n_a e_a, n_a \in \mathbb{Z}\},^{2} \tag{1.1}$$

is then called a lattice, cf. (Pitteri and Zanzotto, 2003, pages 61-62).

The crystal structure is usually characterized by the point group of symmetry $G(e_a)$ of its lattice defined as

$$G(e_a) = \{H \in \mathrm{O}(d), L(He_a) = L(e_a)\}, \tag{1.2}$$

where $\mathrm{O}(d)$ denotes the set of all orthogonal tensors. If the group of symmetry is larger, the crystalline structure is said to be more symmetric and vice versa.

As already announced, a typical SMA exhibits two kinds of crystalline structures: a more symmetric one, the *austenitic* structure and a less symmetric one, the *martensitic* structure; it is of key importance that the martensitic point group of symmetry is a subgroup of the astenitic one Bhattacharya et al. (2004). In some SMAs, like in *NiTi*, even a third structure can be observed; in *NiTi* this is the so-called R-phase (cf. (Šittner et al., 2004)).

In SMAs the *austenitic* structure is usually of a *cubic* symmetry, while the *martensitic* structures can have e.g. a tetragonal (*NiMgGa*, cf. (Bhattacharya, 2003; Kružík and Roubíček, 2004)), an orthorhombic (*CuAlNi*, cf. (Bhattacharya, 2003; Kružík et al., 2005)), a rhombohedral (R-phase of *NiTi*, cf. (Hane and Shield, 2000; Šittner et al., 2004)) or a monoclinic (martensite of *NiTi*, cf. (Bhattacharya, 2003)) symmetry.

Since, in this work, we shall be concerned only with models of SMAs that operate on the continuum mechanics level, we need to transform the description of the austenitic and martensitic phases by crystalline structure to continuum mechanics. Before doing so, let us review some basic kinematic concepts in continuum mechanics we will need to use.

In continuum mechanics one assumes[3] that the investigated body is exposed to an action of forces or displacements on the boundary, which cause a mechanical response characterized by a vectorial function called *deformation*.

Indeed, having a body occupying the domain $\Omega \subset \mathbb{R}^d$ in the reference configuration (in this work the stress-free austenitic state is always assumed to be the reference configuration), any smooth injective function $y(t) : \Omega \to \mathbb{R}^d$ such that $\det \nabla y(x,t) > 0$ is called a *deformation* of the body.

In solids, as in the situation considered in this work, the deformation gradient, ∇y, is often used as the main variable describing the state of the material (Gurtin, 1982). We shall hence assign appropriate deformation gradients to the respective crystalline structures. First of all, we identify the reference austenitic configuration, where the atoms of the body are organized in a lattice $L(e_a^0)$, with the identity matrix, $\mathbb{I} \in \mathbb{R}^{d\times d}$. If then these atoms are rearranged to a lattice $L(e_a)$, e.g. by transforming to martensite, we may assume that the effect is the same as if a homogeneous deformation, the deformation gradient, F, of which satisfies $Fe_a^0 = e_a$, had been applied. This assumption is backed by the so-called *Cauchy-Born hypothesis* (cf. (Bhattacharya, 2003,

[2] Recall that d is the dimension of the problem.

[3] For an introduction to continuum mechanics we refer to e.g. (Gurtin, 1982).

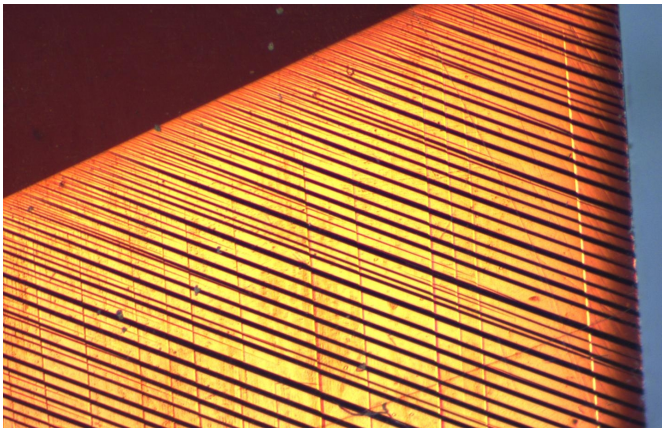


Figure 1.1: Micrograph of the microstructure observed in the SMA *CuAlNi. Courtesy of Hanuš Seiner, LUM, Institute of Thermomechanics of the ASCR.*

pages 34-37)). Therefore, we assign to a martensitic structure with the crystall lattice $L(e_a)$ exactly this matrix F and will use $L(e_a)$ and F interchangeably to describe the martensitic structure.

Now, due to the lower symmetry of the martensitic crystalline structure, several matrices F^i, such that $F^i \neq QF^j$ for any rotation $Q \in \mathrm{SO}(d)$, can be found that transform the austenitic into a martensitic lattice with the prescribed symmetry. These matrices characterize so-called *variants* of martensite. To see this clearer, consider a simple example of a shape memory alloy having a cubic crystalline structure in austenite and tetragonal in martensite. Then, we can form a (martensitic) cuboid by stretching the (austenitic) cube along one arbitrary axis of the coordinate system. All these stretches (described by appropriate deformation gradients U_i) realize the transformation from a cubic to a tetragonal lattice; notice that no $Q \in \mathrm{SO}(d)$ exists such that $U_i = QU_j$. Hence, though there is only one *martensitic phase*, we identified d *variants of martensite.* [4]

It can be observed (cf. e.g. (Bhattacharya, 2003; Pitteri and Zanzotto, 2003) and also Figure 1.1) that variants of martensite can be combined into so-called *twins* or *laminates*. This refers to an arrangement two variants of martensite characterized by matrices U_1 and U_2 into narrow stripes like in Figure 2.1. This kind of *microstructure* is often formed to minimize the elastic energy (see Example 2.20 in Chapter 2). However, such stripes can only be formed between variants characterized by matrices that satisfy

$$U_1 - QU_2 = \mathbf{a} \otimes \mathbf{n},$$

for some vectors $\mathbf{a}$ and $\mathbf{n}$ and some $Q \in \mathrm{SO}(d)$. This condition assures that it is possible to form a planar interface between the two variants in such a way that the overall deformation is continuous; note that $\mathbf{n}$, in particular, is the normal of the interface. We shall elaborate the formation of microstructure in more detail in Chapters 2 and 4. Yet, only the knowledge about the existence of microstructure and twinning allows us to explain, from the microscopic point of view, the most prominent stress-temperature responses observed in SMAs.

To explain the *shape-memory effect* suppose that the specimen is held at a temperature $\theta < \theta_{\mathrm{tr}}$, in martensite, in stress-free configuration. Assume, moreover, that inside

[4] Occasionally in mathematical literature (e.g. (Kružík et al., 2005)), the name "phases" is also used for variants of martensite; in this thesis we might use this nomenclature only when there is no risk of confusion.

the specimen a microstructure, e.g a laminate, has formed. Usually, a SMA specimen is capable to form this microstructure in such a way that the overall (stress-free) shape of the specimen is the same as the shape of the (stress-free) austenite - assume therefore that the material is in this special state. When being deformed by a (suitable) small enough loading the deformation can be compensated by rearrangement of variants and a change in microstructure (cf. (Bhattacharya, 2003, pages 143-150)). On heating, a phase transition to austenite occurs; yet since there is only one variant of austenite there is only one possible shape it can have in a stress free configuration. Therefore the specimen will recover exactly this shape.

In the *superelastic* regime the specimen is held at a temperature $\theta > \theta_{\text{tr}}$; hence the specimen is in the austenitic state. When (suitable) mechanical loads are applied, it transits to martensite and creates a microstructure. The mechanical loads will first induce the phase transition and then force a change in microstructure as described in the case of the shape-memory effect. After removing all loads the only stable stress free configuration at the given temperature is the austenitic one and therefore the material recovers its original shape, similarly as if the material were elastic. (see also (Huo et al., 1994))

Pseudo-plasticity on the other hand occurs when $\theta < \theta_{\text{tr}}$ and mechanical loading is applied. Similarly to the previous cases, the deformation leads to a rearrangement of variants. When all loads are released the new microstructure is stable as well, so the shape of the material is unchanged. Therefore, the behavior of the material seems to be plastic.

1.3 Overview of modeling approaches in the case of SMAs

Of course, modeling the behavior of SMAs is crucial for optimizing their usage in technical systems and hence has received a large amount of attention from mathematicians (cf. e.g. (Arndt et al., 2006; Ball and James, 1987; Dolzmann, 2003; Kružík et al., 2005; Mielke et al., 2009; Mielke and Roubíček, 2003; Paoli and Petrov, 2011; Roubíček, 2004; Roubíček et al., 2007)) as well as engineers (cf. e.g. (Auricchio and Petrini, 2004; Auricchio et al., 2007; Hartl and Lagoudas, 2009; Hartl et al., 2010; Khandelwal and Buravalla, 2009; Lagoudas et al., 2011; Lexcellent et al., 2006; Panico and Brinson, 2007; Souza et al., 1998)) in the past decades. Mathematically correct and accurate models are also highly desired by physicists to help them with interpretation of measured data.

Clearly, modeling the response of SMAs is really a *multiscale* problem. Depending on the purpose of the model, one can approach the description of SMA behavior on different scales ranging from the nano-scale considering only several hundreds of atoms to truly macroscopic models for polycrystalline materials (Roubíček, 2004); cf. also Figure 1.3. Naturally, the larger sizes of the specimen the model considers, the larger is the amount of phenomenology entering the model.

In Figure 1.3 several representative modeling scales are depicted; let us now describe them in more detail.

- Models on the *atomic level* or *nanoscale* use *molecular dynamics* to predict the behavior of the specimen, cf. e.g. (Entel et al., 2000; Meyer and Entel, 1998; Rubini and Ballone, 1995); thus they are able to model only small grains of the size of several nm. For results on mathematical analysis on this scale, we refer to e.g. (Schwetlick and Zimmer, 2007).

- Scales about 1-100 μm will be considered as the *microscopic level* in this work. At this level, it is appropriate to use continuum mechanics as the modeling framework and thus deformation gradients as well as, if necessary, temperature fields are used

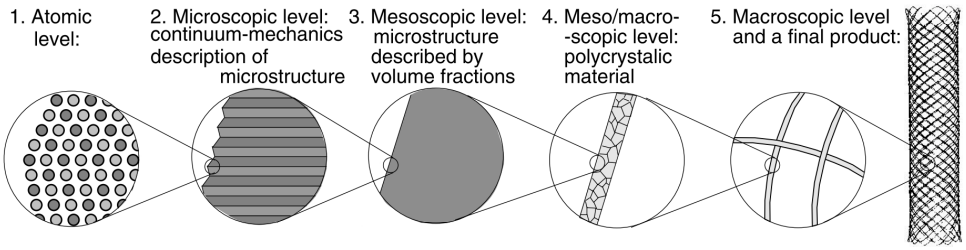


Figure 1.2: A schematic representation of the different scales of an SMA taken from (Roubíček, 2004).

to describe the state of the material. It is characteristic for this scale that the microstructure inside the specimen needs to be fully resolved at this level. Works considering microscopic models include e.g. (Arndt et al., 2006; Aubry et al., 2003; Bhattacharya and James, 1999; Stupkiewicz and Petryk, 2002, 2004, 2010).

- The *mesoscopic* scale is suitable for modeling responses of single crystals of SMA (i.e. at the mm- or cm-scale). At this level, it is again appropriate to use continuum mechanics; however, unlike in microscopic models, the state of the material is described only by "averaged" microscopic deformation gradients (the appropriate mathematical tool are *(gradient) Young measures*, cf. Chapter 2) and volume fractions of the corresponding phases. The modeling assumptions characterizing this scale are given in more detail in Chapter 4; there also the existing literature is reviewed.

- The so-called macroscale is used to model polycrystalline specimen, again in the size of cm. Models on this scale are rather phenomenological and use adequate internal variables (like the vector of volume fractions of martensite and the transformation strain, see e.g. (Sedlák et al., 2012)) to describe the state of the specimen. Constitutive equations are chosen in such a way, that the model reproduces thermal/mechanical loading cycles; often some parameters need to be fitted. A non-exhaustive list of macroscopic models proposed in the past years includes (Auricchio et al., 2007; Bernardini and Pence, 2002; Frost et al., 2010; Hartl and Lagoudas, 2009; Hartl et al., 2009; Lagoudas et al., 2011; Lexcellent et al., 2000; Panico and Brinson, 2007; Patoor et al., 2006; Rajagopal and Srinivasa, 1999; Sedlák et al., 2010; Souza et al., 1998).

One of the biggest challenges in mathematical modeling is not only to analyze the models on every individual scale, but also to *rigorously prove* a scale transition between the respective models, when, due to the increased size of the specimen, some quantities become negligible and/or the response corresponds to a homogenized structure (Patoor, 2009; Roubíček, 2004). As far as the transition from the nanoscale to the microscopic scale is concerned, so far, only very few results on a *rigorous scale transition* between these two levels are given in literature (Zimmer, 2006), one of the pioneering works aiming however to plasticity rather then SMAs is (Mielke and Truskinovsky, 2012).

As to the transition between the microscopic and mesoscopic models, note, that in this work we *rigorously prove* that the description on the mesoscopic level can be seen as a *limit of microscopic models* when the surface energy of twin boundaries and/or austenite/martensite interface becomes negligible compared to the total stored energy of the specimen, cf. Chapter 5. While this is fairly easy to establish in the static case (see Proposition 4.1), in Theorem 5.12 we prove a (formalized version) of this statement also in thermally coupled case.

The scale transition from the micro/mesoscopic level to the macroscopic level seems to be very hard not only from the mathematical but also from the physical point of view - e.g. the precise influence of texture of the material on its overall behavior is still not explored well enough; it could be based on some statistical approach as in (Bruno et al., 1996).

Chapter 2

Mathematical background on relaxation of variational problems

In this chapter we shall review some basic mathematical concepts on relaxation in calculus of variations. To this end, let us define the functional $I : W^{1,p}(\Omega;\mathbb{R}^d) \to \mathbb{R}$ as

$$I(y) = \int_\Omega \phi(\nabla y)\,\mathrm{d}x, \tag{2.1}$$

and we shall be concerned with the problem

$$\left.\begin{array}{ll} \text{Minimize} & I(y) \\ \text{subject to} & y \in W^{1,p}_{\Gamma_\mathrm{D}}(\Omega,\mathbb{R}^d), \end{array}\right\} \tag{2.2}$$

with $\Gamma_\mathrm{D} \subset \partial\Omega$, Ω a regular domain, $W^{1,p}_{\Gamma_\mathrm{D}}(\Omega,\mathbb{R}^d) = \left\{W^{1,p}(\Omega;\mathbb{R}^d) \text{ with } y = x \text{ on } \Gamma_\mathrm{D}\right\}$ (cf. also the Nomenclature) and ϕ a *continuous* function[1], usually of p-growth, i.e.

$$c_1(|F|^p - 1) \leq \phi(F) \leq c_2(1 + |F|^p), \tag{2.3}$$

for some $c_1, c_2 > 0$.

In Section 2.2 we shall first state under which assumptions on ϕ one can guarantee existence of solutions to (2.2), i.e. we introduce quasiconvexity. Also, we introduce upper and lower bounds for the quasiconvex envelope. In Section 2.3.1 we introduce (gradient) Young measures and state their basic properties. Finally, in Section 2.3.2, we introduce a recent characterization of a special subset of Young measures, that, when used for relaxation, allows for a generalization of the constraint (2.3) on ϕ.

Let us note that, since this chapter is understood as an introductory review, we give the majority of theorems without proofs and only refer to literature.

2.1 Basic notation

Before starting the review in the next sections, let us fix, at this point, some notation we shall use hereinafter.[2]

As already announced in the Nomenclature, if not specified differently, the exponent p takes values in $(1,\infty)$, i.e. excluding 1 and ∞.

[1] We do not consider ϕ dependent on x; however all of theorems stated here have been generalized also to this case if ϕ is a *Carathédory function*; cf. (Benešová, Kružík and Pathó, 2012; Dacorogna, 1989; Pedregal, 1997)

[2] Let us remind the reader that some basic notation has also been summarized in the Nomenclature at the beginning of this thesis.

Standardly, $C_0(\mathbb{R}^{d\times d})$ denotes for the space of all continuous functions on $\mathbb{R}^{d\times d}\to\mathbb{R}$ vanishing at infinity, hence $C_0(\mathbb{R}^{d\times d})=\overline{C_c(\mathbb{R}^{d\times d})}$ with $C_c(\mathbb{R}^{d\times d})$ the space of continuous functions with compact support. By the classical Riesz theorem (see e.g. the monograph (Rudin, 1991)) its dual $C_0(\mathbb{R}^{d\times d})^*$ is isometric isomorph to the space of Radon measures $\mathcal{M}(\mathbb{R}^{d\times d})$, normed by the total variation. We shall denote by $L^\infty_{\rm w}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d}))$ the space of essentially bounded weakly* measurable mappings $x\mapsto\nu_x:\Omega\to\mathcal{M}(\mathbb{R}^{d\times d})$; the adjective "weakly* measurable" means that, for any $v\in C_0(\mathbb{R}^{d\times d})$, the mapping $\Omega\to\mathbb{R}:x\mapsto\langle\nu_x,v\rangle=\int_{\mathbb{R}^{d\times d}}v(s)\nu_x(\,{\rm d}s)$ is measurable in the usual sense.

Let us also introduce continuous functions with "sub-p growth" as

$$C_p(\mathbb{R}^{d\times d}):=\left\{v\in C(\mathbb{R}^{d\times d});\ \lim_{|s|\to\infty}\frac{v(s)}{|s|^p}=0\right\}\ .$$

Eventually, we shall also need continuous functions with an appropriate growth defined only on invertible matrices $\mathbb{R}^{d\times d}_{\rm inv}$

$$C_{p,-p}(\mathbb{R}^{d\times d}_{\rm inv}):=\left\{v\in C(\mathbb{R}^{d\times d}_{\rm inv});\ \lim_{|s|+|s^{-1}|\to\infty}\frac{v(s)}{|s|^p+|s^{-1}|^p}=0\right\}\ . \tag{2.4}$$

2.2 Quasiconvexity, polyconvexity and rank-one convexity

To formalize ideas, let us take I from (2.1) with ϕ continuous, satisfying (2.3) and $p\in(1,\infty)$.

As highlighted above, we are to investigate existence of minima; a convenient method of proving that I possesses at least one minimizer is the so-called *direct method* which works as follows: Take $\{y_k\}_{k=0}^\infty$, an infimizing sequence of the functional I, which, due thanks to (2.3) (*coercivity*), will be bounded in $W^{1,p}(\Omega,\mathbb{R}^d)$. Hence, due to the reflexivity of Sobolev spaces for $p\in(1,\infty)$, a subsequence of $\{y_k\}_{k=0}^\infty$ (not-relabeled) converges weakly to y in $W^{1,p}(\Omega,\mathbb{R}^d)$. If I were *(sequentially) weakly lower semi-continuous* on $W^{1,p}(\Omega,\mathbb{R}^d)$ [3] then clearly y would be the sought minimizer - i.e. *weak lower semi-continuity* is a *sufficient property* for I to have minimizer. Therefore, we shall concentrate on studying this property; in fact we shall see that, provided (2.3), I is weakly lower semi-continuous *if and only if* it is *quasiconvex* (cf. Definition 2.1 and Proposition 2.2).

Definition 2.1. [4] We say that a continuous $\varphi:\mathbb{R}^{d\times d}\to\mathbb{R}$ is *quasiconvex* in $Y\in\mathbb{R}^{d\times d}$ if

$$\varphi(Y)\le\inf_{\omega\in W^{1,\infty}_0(\Omega,\mathbb{R}^d)}\frac{1}{|\Omega|}\int_\Omega\varphi(Y+\nabla\omega)\,{\rm d}x. \tag{2.6}$$

A function φ quasiconvex in Y is called $W^{1,p}$*-quasiconvex* if moreover

$$\varphi(Y)\le\inf_{\omega\in W^{1,p}_0(\Omega,\mathbb{R}^d)}\frac{1}{|\Omega|}\int_\Omega\varphi(Y+\nabla\omega)\,{\rm d}x. \tag{2.7}$$

The function φ is called simply ($W^{1,p}$-)quasiconvex if it is ($W^{1,p}$-)quasiconvex in all $Y\in\mathbb{R}^{d\times d}$.

[3] I is *(sequentially) weakly lower semi-continuous* on $W^{1,p}(\Omega,\mathbb{R}^d)$ if, for any sequence $y_k\rightharpoonup y$ in $W^{1,p}(\Omega,\mathbb{R}^d)$,

$$I(y)\le\liminf_{k\to\infty}I(y_k). \tag{2.5}$$

[4] The notion of quasiconvexity was introduced by Morrey (1952), the generalized concept of $W^{1,p}$-quasiconvexity was later introduced by Ball and Murat (1984).

Proposition 2.2. [5] *Let $\phi : \mathbb{R}^{d\times d} \to \mathbb{R}$ be a continuous function satisfying (2.3) for every $F \in \mathbb{R}^{d\times d}$ and $p \in (1,\infty)$. Then the I defined through (2.1) is weakly lower semi-continuous if and only if ϕ is quasiconvex.*

If ϕ in (2.1) fails to be quasiconvex, existence of solutions (2.2) to usually cannot be established by the direct method; often, even non-existence of minima is a consequence. In this situation, therefore, we need to find a *relaxation* of the original problem.

Definition 2.3. [6] Take a functional $I : V \to \mathbb{R}$, with V a linear vector space. Further, let us take a linear vector space X on which a notion of convergence is defined. Then we call the functional $\tilde{I} : X \to \mathbb{R}$ is called a relaxation of I, if

1. $V \subset X$, or if at least V can be identified with a subset of X through an isomorphism,
2. there exists $\tilde{x} \in X$ satisfying $\tilde{I}(\tilde{x}) = \min_{x\in\overline{V}^X} \tilde{I}(x)$ with $\overline{V}^X$ denoting the closure of V with respect to the convergence on X,
3. any cluster point of an infimizing sequence to I, with respect to the convergence on X, satisfies that $\tilde{I}(\bar{x}) = \min_{x\in\overline{V}^{\|\cdot\|_X}} \tilde{I}(x)$.
4. for any $\tilde{x} \in X$ such that $\tilde{I}(\tilde{x}) = \min_{x\in\overline{V}^X} \tilde{I}(x)$ there exists a minimizing sequence of I that converges to $\tilde{x}$.

In order to define relaxations of I from (2.1) with ϕ not quasiconvex we introduce the *quasiconvex* envelope of ϕ through

$$Q\phi(Y) = \sup\left\{\varphi(Y); \varphi \text{ quasiconvex}, \varphi(F) \le \phi(F) \text{ for all } F \in \mathbb{R}^{d\times d}\right\}, \quad [7] \tag{2.8}$$

and define the following functional

$$I^*(y) = \int_\Omega Q\phi(\nabla y)\,\mathrm{d}x. \tag{2.9}$$

As shown by the following proposition, $I^*(y)$ is then a *relaxation* of $I(y)$:

Proposition 2.4. [8] *Take I from (2.1) with ϕ continuous, satisfying (2.3). Then there exists a minimizer of I^* on $W^{1,p}_{\Gamma_D}(\Omega,\mathbb{R}^d)$ and*

$$\min_{y\in W^{1,p}_{\Gamma_D}(\Omega,\mathbb{R}^d)} I^*(y) = \inf_{y\in W^{1,p}_{\Gamma_D}(\Omega,\mathbb{R}^d)} I(y).$$

Moreover, any cluster point of an infimizing sequence $\{y_k\}_{k\in\mathbb{N}}$ in $W^{1,p}_{\Gamma_D}(\Omega,\mathbb{R}^d)$ minimizes I^* and vice versa any minimizer of I^* is a cluster-point of a infimizing sequence of I.

[5] This proposition is essentially due to Morrey (1952). Actually, if (2.3) is fulfilled, ϕ is even $W^{1,p}$-quasiconvex; so, we could equivalently demand ϕ to be also $W^{1,p}$-quasiconvex as shown by (Ball and Murat, 1984).

[6] Note that the definition of relaxation given is very general in order to able to cope also with relaxation by Young measures.

[7] If ϕ is a locally bounded continuous function the quasiconvex envelope can also be defined as (see e.g. (Dacorogna, 1989, Section 5.1.1.2))

$$Q\phi(Y) = \inf_{\omega\in W^{1,p}_0} \frac{1}{|\Omega|}\int_\Omega \phi(Y+\nabla\omega)\mathrm{d}x.$$

[8] This is originally due to Dacorogna (1989, Section 1), here taken from (Pedregal, 1997).

Remark 2.5. An important property that allows us to prove that I^* really possesses minimizers is the fact that the growth of ϕ (2.3) is preserved also for its quasiconvex envelope (Dacorogna, 1989); in particular, the coercivity is preserved, which allows us to extract a weakly converging subsequence out of the infimizing sequence.

Hence, we have found a suitable relaxation of I (from 2.1) through calculating the convex hull of ϕ. Yet, even if we could use the formula

$$Q\phi(Y) = \inf_{\omega \in W_0^{1,p}} \frac{1}{|\Omega|} \int_\Omega \phi(Y + \nabla\omega) \mathrm{d}x,$$

to do so, we had to *explicitly* solve yet another minimization problem, that we are, mostly, unable to do. Therefore, it is desirable to replace, e.g. in numerical calculations, the quasiconvex hull by some kind of its approximation; two approximations are commonly used: the *polyconvex* hull and the *rank-1 convex* hull. To introduce these two, let us first define *rank-1 convex* and *polyconvex* functions.

Definition 2.6 (Polyconvexity)**.** [9] We say that a function $\varphi : \mathbb{R}^{d\times d} \to \mathbb{R}$ is polyconvex if there exist another function $\psi : \mathbb{R}^{d\times d} \times \mathbb{R}^{d\times d} \times \mathbb{R} \mapsto \mathbb{R}$ that is *convex* such that

$$\varphi(A) = \psi(A, \mathrm{cof}(A), \det(A)).$$

Definition 2.7 (Rank-1 convexity)**.** [10] We say that $\varphi : \mathbb{R}^{d\times d} \to \mathbb{R}$ is rank-1 convex if

$$\phi(\lambda F_1 + (1-\lambda)F_2) \leq \lambda\phi(F_1) + (1-\lambda)\phi(F_2). \tag{2.10}$$

for all $\lambda \in [0,1]$ and all F_1, F_2 such that $\mathrm{rank}(F_1 - F_2) \leq 1$

Having Definitions 2.6 and 2.7 at hand, the polyconvex envelope of ϕ is, analogously to (2.8), defined through

$$P\phi = \sup\left\{\varphi(Y); \varphi \text{ polyconvex}, \varphi(F) \leq \phi(F) \text{ for all } F \in \mathbb{R}^{d\times d}\right\}, \tag{2.11}$$

whereas the rank-1 convex envelope of ϕ is defined analogously through

$$P\phi = \sup\left\{\varphi(Y); \varphi \text{ rank-1 convex}, \varphi(F) \leq \phi(F) \text{ for all } F \in \mathbb{R}^{d\times d}\right\}. \tag{2.12}$$

Due to the general relation

$$\text{convexity} \Rightarrow \text{polyconvexity} \Rightarrow \text{quasiconvexity} \Rightarrow \text{rank-1 convexity}, \tag{2.13}$$ [11]

we find that for the envelopes and their minimizers/infimizers the following relations holds

$$P\phi \leq Q\phi \leq R\phi \leq \phi, \tag{2.14}$$

$$\min_{v\in V} \int_\Omega P\phi(x,v)\mathrm{d}x \leq \min_{v\in V} \int_\Omega Q\phi(x,v)\mathrm{d}x = \inf_{v\in V} \int_\Omega R\phi(x,v)\mathrm{d}x = \inf_{v\in V} \int_\Omega \phi(x,v)\mathrm{d}x, \tag{2.15}$$

[9] The notion of polyconvexity was introduced by Ball (1977).

[10] The notion of rank-1 convexity was introduced by Morrey (2008).

[11] This can be found e.g. in (Dacorogna, 1989). Note that none of the converse implications holds if $\phi : \mathbb{R}^{d\times d} \to \mathbb{R}$ and $d > 2$ (while for $d = 1$ all implications are in fact equivalences). To see that polyconvexity does not imply convexity (even for $d > 1$) just consider the function $\phi(F) = \det(F)$ which is even polyaffine but not convex. Also quasiconvexity does not imply polyconvexity even for $d > 1$ as was shown in e.g. (Dacorogna, 1989). Šverák's important counter example (Šverák, 1992) is a construction of a function that is rank-1 convex, but not quasiconvex and holds for $d > 3$. For $d = 2$ the question whether quasiconvexity and rank-1 are equivalent is still open.

with $V = W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^d)$.

Therefore, working with the polyconvex envelope (as an *estimation* of the quasiconvex one) can lead to *under-relaxation* of the problem, i.e. the energy corresponding to the found minimizer is too small. On the other hand, working with the rank-1 convex envelope bears the drawback that for it the existence of minimizers cannot be guaranteed.

Nevertheless, both the polyconvex and the rank-1 convex envelope have the advantage that they can be, at least in some approximation, calculated numerically. Moreover, the infimum of the rank-1 convex envelope gives the same value as the minimum of the quasiconvex one. Of course the supremum definitions (2.11) - (2.12) are not suitable to do so, since they are not explicit; however for the rank-1 convex envelope we can exploit Proposition 2.8[12] while for the polyconvex envelope so-called polyconvex measures (see Definition 2.17 and (Bartels and Kružík, 2011)) can be employed.

Indeed for the rank-1 convex envelope we have:

Proposition 2.8. [13] *Let $\varphi : \mathbb{R}^{d\times d} \to \mathbb{R}$ be bounded from below. Then for any $F \in \mathbb{R}^{d\times d}$ it holds that*

$$\begin{aligned} R\varphi(F) &= \lim_{k\to\infty} R_k\varphi(F) \quad \text{where} \\ R_0\varphi &= \varphi \quad \text{and} \\ R_{k+1}\varphi F &= \inf\{\lambda R_k\varphi(F_1) + (1-\lambda)R_k\varphi(F_2), \text{ where } \lambda \in [0,1] \\ &\qquad \text{such that } F = \lambda F_1 + (1-\lambda)F_2 \text{ and } \operatorname{rank}(F_1 - F_2) \le 1\}. \end{aligned}$$

Let us note that the procedure (and the closely related concept of laminates in Definition 2.15) from Proposition 2.8 shall be exploited in numerical implementations in Chapter 7; in numerics then we use only some $R_k\varphi$ to approximate $R\varphi$.

To sum up this subsection, *quasiconvexity* (cf. Definition 2.1) of the function ϕ is, under growth condition (2.3), a necessary and sufficient condition for weak lower semi-continuity of the functional I from (2.1); this (again thanks to (2.3)) implies the existence of minimizers. Should ϕ not be quasiconvex we can relax the functional by substituting ϕ by its quasiconvex envelope (see 2.8). Yet, this envelope is hard to compute and hence it is approximated by the polyconvex (2.11) or rank-1 convex (2.12) envelope.

2.3 (Gradient) Young measures

Though replacing ϕ in I from (2.1) by its quasiconvex envelope is a straightforward way of relaxation for minimization problems, its main drawback is that a lot of information about the behavior of infimizing sequences of the original problem is lost. Therefore, we introduce an equivalent tool, *gradient Young measures*, that assures existence of minimizers, but, on the other hand, also keeps track about some important features of the infimizing sequences.

Young measures were introduced by Young in the connection with optimal control (Young, 1937) and studied by many authors in different contexts later. Some of the results given here can be found e.g. in (Ball, 1989; Fonseca and Kružík, 2010; Fonseca and Leoni, 2007; Fonseca et al., 1998; Kinderlehrer and Pedregal, 1991, 1992, 1994; Kristensen, 1994; Kružík and Roubíček, 1996; Pedregal, 1997; Valadier, 1990) and many others; for introductory reading e.g. the monographs (Fonseca and Leoni, 2007; Pedregal, 1997) are suitable.

[12] Or, equivalently, we could work with so-called laminates, cf. Definition 2.15.

[13] This can be found e.g. in (Kohn and Strang, 1986) or (Dacorogna, 1989, Section 5.1)

2.3.1 General facts on (gradient) Young measures

We shall start this section by giving the fundamental theorem introducing Young measures:

Theorem 2.9. [14]

1. *Let $\{u_k\}_{k=0}^{\infty}$ be a bounded sequence in $L^\infty(\Omega,\mathbb{R}^{d\times d})$ (i.e. $u_k(x)\in K$ with $K\subset\mathbb{R}^{d\times d}$ compact for a.a. $x\in\Omega$ and all $k\in\mathbb{N}$). Then there exists a subsequence of $\{u_k\}_{k=0}^{\infty}$ (not relabeled) and a family of probability measures $\nu=\{\nu_x\}\subset L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d}))$[15] with the property that for any continuous function $\phi:\mathbb{R}^{d\times d}\to\mathbb{R}$*

$$\lim_{k\to\infty}\int_\Omega \xi(x)\phi(u_k(x))\mathrm{d}x=\int_\Omega \xi(x)\int_{\mathbb{R}^{d\times d}}\phi(A)\mathrm{d}\nu_x(A)\mathrm{d}x, \tag{2.16}$$

for any $\xi\in L^\infty(\Omega)$. Moreover, $\operatorname{supp}\nu_x\subset K$ for a.a. $x\in\Omega$.

2. *Let $\{u_k\}_{k=0}^{\infty}$ be a bounded sequence in $L^p(\Omega,\mathbb{R}^{d\times d})$ for some $p\in(1,\infty)$. Then there exists a subsequence of $\{u_k\}_{k=0}^{\infty}$ (not relabeled) and a family of probability measures $\nu=\{\nu_x\}\subset L^\infty_{\mathrm{w}}(\Omega;\mathrm{rca}(\mathbb{R}^{d\times d}))$ with the property that for any continuous function $\phi:\mathbb{R}^{d\times d}\to\mathbb{R}$ such that $\{\phi(u_k(x))\}_{k=0}^{\infty}$ is weakly convergent in $L^1(\Omega)$ (2.16) holds.*
   In particular, if $\phi\in C_p(\mathbb{R}^{d\times d})$ then the condition of weak convergence on ϕ in $L^1(\Omega)$ is satisfied.

For shortening the notation, let us introduce the "momentum" operator " $\bullet$ " defined by

$$[f\bullet\nu](x):=\int_{\mathbb{R}^{d\times d}} f(s)\nu_x(\mathrm{d}s). \tag{2.17}$$

In view of Theorem 2.9 we introduce the set of *Young measures*

$$\mathscr{Y}(\Omega;\mathbb{R}^{d\times d})=\Big\{\nu\in L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d}));\ \exists\{u_k\}_{k=0}^{\infty}\subset L^\infty(\Omega,\mathbb{R}^{d\times d})\ \text{s.t.}$$
$$\int_\Omega\xi(x)\phi(u_k)\,\mathrm{d}x\to\int_\Omega\xi(x)\phi\bullet\nu\,\mathrm{d}x\ \text{for all}\ \xi\in L^\infty(\Omega),\phi\in C(\mathbb{R}^{d\times d})\Big\}\,, \tag{2.18}$$

as well as the set of *L^p-Young measures*

$$\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d})=\Big\{\nu\in L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d}));\ \exists\{u_k\}_{k=0}^{\infty}\subset L^p(\Omega,\mathbb{R}^{d})\ \text{s.t.}$$
$$\int_\Omega\xi(x)\phi(u_k)\,\mathrm{d}x\to\int_\Omega\xi(x)\phi\bullet\nu\,\mathrm{d}x\ \text{for all}\ \xi\in L^\infty(\Omega),\phi\in C_p(\mathbb{R}^{d\times d})\Big\}\,, \tag{2.19}$$

Take any (L^p-)Young measure ν. Then the sequence $\{u_k\}_{k=0}^{\infty}$ for which (2.16) holds is called a *generating* sequence of ν and, on the other hand, ν is called the Young measure *associated* to $\{u_k\}_{k=0}^{\infty}$.

A characterization of the sets $\mathscr{Y}$ and $\mathscr{Y}^p$ posing only requirements on the involved measures themselves is given through Proposition 2.10:

Proposition 2.10. [16]

- *$\nu\in L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d}))$ is an element of $\mathscr{Y}(\Omega;\mathbb{R}^{d\times d})$ if and only if $\operatorname{supp}\nu_x\subset K$ for some compact set K for a.a. $x\in\Omega$.*

[14] In the L^∞ case we refer to (Tartar, 1995; Warga, 1972), for the L^p case this was for the first time shown by Schonbek (1982); for a proof we may point the reader also to e.g. (Ball, 1989).

[15] In the sequel, we shall often omit the index x for ν and have the whole family in mind.

[16] For $\mathscr{Y}$ and $\mathscr{Y}^p$ we refer to (Valadier, 1990) and (Kružík and Roubíček, 1996), respectively.

- $\nu \in L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d}))$ *is an element of* $\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d})$ *if and only if* $\int_\Omega |\cdot|^p \bullet \nu \,\mathrm{d}x < +\infty$.

Suppose that $\{u_k\}_{k=0}^\infty \subset L^p(\Omega,\mathbb{R}^d)$ is a generating sequence for the measure $\nu \subset \mathscr{Y}^p(\Omega;\mathbb{R}^d)$. Then, for continuous ϕ satisfying only (2.3) (and thus no necessarily elements of $C_p(\mathbb{R}^{d\times d})$), the relation (2.16) does *not* follow from Theorem 2.9 and does not even need to be true in general. [17] However, at least an inequality by the following proposition can be established.

Lemma 2.11. [18] *Let φ be an arbitrary continuous function bounded from below, $\{z_k\}_{k=1}^\infty$ a bounded sequence in $L^p(\Omega,\mathbb{R}^{d\times d})$ and $\nu = \{\nu_x\}$ the associated gradient Young measure. Then*

$$\int_\Omega \varphi \bullet \nu \,\mathrm{d}x \le \liminf_{k\to\infty} \int_\Omega \varphi(z_k)\mathrm{d}x. \tag{2.20}$$

Remark 2.12. It follows from the proof Proposition 2.10 given in (Kružík and Roubíček, 1996) that for any $\nu \in \mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d})$ there *exist at least one generating sequence* of ν denoted $\{\tilde z_k\}_{k=1}^\infty$ such that $|\tilde z_k|^p$ is weakly convergent in $L^1(\Omega)$.

In particular this means that, for this sequence $\{\tilde z_k\}_{k=1}^\infty$, and for any continuous ϕ satisfying *only* (2.3) we even have that

$$\int_\Omega \phi \bullet \nu \,\mathrm{d}x = \lim_{k\to\infty} \int_\Omega \phi(\tilde z_k)\,\mathrm{d}x.$$

An important subclass of (L^p-)Young measures are those generated by gradients of functions in $W^{1,\infty}(\Omega;\mathbb{R}^d)$ or $W^{1,p}(\Omega;\mathbb{R}^d)$ called (L^p-)*gradient Young measures* - let us, thus, define those subclasses as:

$$\begin{aligned}\mathscr{G}(\Omega;\mathbb{R}^{d\times d}) := \Big\{&\nu \in L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d})); \exists \{u_k\}_{k=0}^\infty \subset W^{1,\infty}(\Omega;\mathbb{R}^d) \text{ s.t.}\\ &\int_\Omega \xi(x)\phi(\nabla u_k)\,\mathrm{d}x \to \int_\Omega \xi(x)\phi\bullet\nu\,\mathrm{d}x \text{ for all } \xi\in L^\infty(\Omega), \phi\in C(\mathbb{R}^{d\times d})\Big\},\end{aligned} \tag{2.21}$$

$$\begin{aligned}\mathscr{G}^p(\Omega;\mathbb{R}^{d\times d}) := \Big\{&\nu \in L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d})); \exists \{u_k\}_{k=0}^\infty \subset W^{1,p}(\Omega,\mathbb{R}^d) \text{ s.t.}\\ &\int_\Omega \xi(x)\phi(\nabla u_k)\,\mathrm{d}x \to \int_\Omega \xi(x)\phi\bullet\nu\,\mathrm{d}x \text{ for all } \xi\in L^\infty(\Omega), \phi\in C_p(\mathbb{R}^{d\times d})\Big\}.\end{aligned} \tag{2.22}$$

For gradient Young measures one could even demand a boundary condition to be satisfied for the generating sequence (in sense of traces); here we shall need only the "identity boundary condition", which corresponds to zero displacement at some part $\Gamma_{\mathrm{D}} \subset \partial\Omega$ of the boundary; i.e. we are interested in

$$\begin{aligned}\mathscr{G}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d}) := \Big\{&\nu \in L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d})); \exists \{u_k\}_{k=0}^\infty \subset W^{1,\infty}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^d) \text{ s.t.}\\ &\int_\Omega \xi(x)\phi(\nabla u_k)\,\mathrm{d}x \to \int_\Omega \xi(x)\phi\bullet\nu\,\mathrm{d}x \text{ for all } \xi\in L^\infty(\Omega), \phi\in C(\mathbb{R}^{d\times d})\Big\},\end{aligned} \tag{2.23}$$

$$\begin{aligned}\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d}) := \Big\{&\nu \in L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d})); \exists \{u_k\}_{k=0}^\infty \subset W^{1,p}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^d) \text{ s.t.}\\ &\int_\Omega \xi(x)\phi(\nabla u_k)\,\mathrm{d}x \to \int_\Omega \xi(x)\phi\bullet\nu\,\mathrm{d}x \text{ for all } \xi\in L^\infty(\Omega), \phi\in C_p(\mathbb{R}^{d\times d})\Big\}.\end{aligned} \tag{2.24}$$

[17] For example consider the sequence

$$u_k(x) = \begin{cases} k & \text{if } x\in[0,1/k^2],\\ 0 & \text{elsewhere,}\end{cases}$$

which is bounded in $L^2([-1,1])$ and generates the Young measure δ_0. Now take $\phi(A) = A^2$. Then clearly $\lim_{k\to\infty}\int_{-1}^1 \phi(u_k)\,\mathrm{d}x = 1$ for all $k\in\mathbb{N}$. Yet, $\int_{-1}^1 \phi\bullet\delta_0\,\mathrm{d}x = 0$.

[18] This lemma is taken from (Pedregal, 1997) and is a consequence of Chacon's biting lemma originally proved by Brooks and Chacon (1980).

Also for the sets of gradient Young measures a characterization has been obtained that poses only requirements on the involved measures themselves and not on the generating sequences. We give this characterization for gradient Young measures in Theorem 2.13 and in Theorem 2.14 for L^p-gradient Young measures.

Theorem 2.13. [19] *Let $\nu = \{\nu_x\} \in L^\infty_{\mathrm{w}}(\Omega; \mathcal{M}(\mathbb{R}^{d\times d}))$ be a family of probability measures. Then $\nu \in \mathscr{G}(\Omega; \mathbb{R}^{d\times d})$ ($\nu \in \mathscr{G}_{\Gamma_{\mathrm{D}}}(\Omega; \mathbb{R}^{d\times d})$) if and only if*

1. *there exists $z \in W^{1,\infty}(\Omega; \mathbb{R}^d)$ ($W^{1,\infty}_{\Gamma_{\mathrm{D}}}(\Omega; \mathbb{R}^d)$) such that $\nabla z = \mathrm{id} \bullet \nu$* [20] *for a.e. $x \in \Omega$,*
2. *$\psi(\nabla z(x)) \leq \psi(A) \bullet \nu_x$ for a.e. $x \in \Omega$ and for all ψ quasiconvex, continuous and bounded from below,*
3. *$\operatorname{supp} \nu_x \subset K$ for some compact set $K \subset \mathbb{R}^{d\times d}$ and a.a. $x \in \Omega$.*

Theorem 2.14. [21] *Let $p \in (1, \infty)$. and let $\nu = \{\nu_x\} \in L^\infty_{\mathrm{w}}(\Omega; \mathcal{M}(\mathbb{R}^{d\times d}))$ be a family of probability measures. Then $\nu \in \mathscr{G}^p(\Omega; \mathbb{R}^{d\times d})$ ($\nu \in \mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega; \mathbb{R}^{d\times d})$) if and only if*

1. *there exists a $z \in W^{1,p}(\Omega; \mathbb{R}^d)$ ($W^{1,p}_{\Gamma_{\mathrm{D}}}(\Omega; \mathbb{R}^d)$) such that $\nabla z = \mathrm{id} \bullet \nu$ for a.e. $x \in \Omega$,*
2. *$\psi(\nabla z(x)) \leq \psi(A) \bullet \nu_x$ for a.e. $x \in \Omega$ and for all ψ quasiconvex, continuous, bounded from below and such that $|\psi(F)| \leq c(1 + |F|^p)$ with $c > 0$,*
3. *$\int_\Omega |\cdot|^p \bullet \nu_x \,\mathrm{d}x < \infty$.*

As will be proved below (cf. Theorem 2.19), L^p-gradient Young measures, characterized by Theorem 2.14, present an appropriate tool of relaxation for problems like in (2.2). Yet, their explicit characterization requires the Jensen inequality (cf. point 2 in Theorem 2.14) to be satisfied for all quasiconvex functions and hence, as it cannot be easily verified whether a function is quasiconvex or not, it cannot be easily verified whether a parameterized measure is indeed in $\mathscr{G}^p(\Omega; \mathbb{R}^{d\times d})$. Therefore, similarly as for the quasiconvex envelope, for numerical calculations we need to replace the set of L^p-gradient Young measures by another suitable set. Two replacements that correspond to the polyconvex and rank-1 convex envelope, respectively (cf. (Bartels and Kružík, 2011) for the polyconvex envelope and e.g. (Pedregal, 1997) for the rank-1 convex one) are possible, we define them

Definition 2.15. The set $\{\lambda_i, F_i\}_{i=1}^{2^l}$ for $\lambda_i > 0$ for all i and $\sum_{i=1}^{2^l} \lambda_i = 1$ is said to satisfy the lamination condition of the l-th order if

1. for $l = 1$ $\operatorname{rank}(F_1 - F_2) \leq 1$,
2. for $l > 1$ (after possibly rearranging indices) $\operatorname{rank}(F_1 - F_2) \leq 1, \operatorname{rank}(F_3 - F_4) \leq 1 \ldots \operatorname{rank}(F_{2^l-1} - F_{2^l}) \leq 1$ and the set $\{\tilde\lambda_i, \tilde F_i\}_{i=1}^{2^{l-1}}$ where

$$\begin{aligned} \tilde\lambda_1 &= \lambda_1 + \lambda_2, & \tilde F_1 &= \tfrac{\lambda_1}{\tilde\lambda_1} F_1 + \tfrac{\lambda_2}{\tilde\lambda_1} F_2 \\ \tilde\lambda_2 &= \lambda_3 + \lambda_4, & \tilde F_4 &= \tfrac{\lambda_3}{\tilde\lambda_2} F_3 + \tfrac{\lambda_4}{\tilde\lambda_2} F_4 \\ &\vdots & &\vdots \\ \tilde\lambda_{2^{l-1}} &= \lambda_{2^l-1} + \lambda_{2^l}, & \tilde F_{2^{l-1}} &= \tfrac{\lambda_{2^l-1}}{\tilde\lambda_{2^l-1}} F_{2^l-1} + \tfrac{\lambda_{2^l}}{\tilde\lambda_{2^l-1}} F_{2^l} \end{aligned}$$

satisfies the lamination condition of order $l - 1$.

[19] This is a result of Kinderlehrer and Pedregal (1991).
[20] Recall that $\mathrm{id} : \mathbb{R}^{d\times d} \to \mathbb{R}^{d\times d}$ is the identity mapping.
[21] This is a result of Kinderlehrer and Pedregal (1994).

Definition 2.16. Let $\{\lambda_i, F_i\}_{i=1}^{2^l}$ be a set that satisfies the lamination condition of the order l. Then the gradient parameterized measure $\nu^l = \sum_{i=1}^{2^l} \lambda_i \delta_{F_i}$, where δ is the Dirac mass, is called a laminate of the l-th order.

The equivalent to the rank-1 convex envelope is then the set of laminates defined as

$$\mathscr{L}^p(\Omega;\mathbb{R}^{d\times d}) = \big\{\nu \in L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d}));\, \exists\, \nu_l \text{ laminates of the } l\text{-th order s.t.} \\ \nu_l \overset{*}{\rightharpoonup} \nu \text{ in } L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d}))\big\}. \tag{2.25}$$

For the equivalent of the polyconvex envelope we introduce the following definition (cf. (Bartels and Kružík, 2011))

Definition 2.17. A parameterized measure $\nu \in L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d}))$ is called *polyconvex* and belongs to the set $\mathscr{P}^p(\Omega;\mathbb{R}^{d\times d})$ if there exists a $y \in W^{1,p}(\Omega;\mathbb{R}^d)$ such that for *a.a.* $x \in \Omega$

$$\mathbb{T}(\nabla y(x)) = \mathbb{T} \bullet \nu,$$

where $\mathbb{T}(F)$ denotes the vector of all subdeterminants of F.

The following relation holds between the set of L^p - gradient Young measures, laminates and the set of polyconvex measures (cf. (Pedregal, 1997) for the first inclusion, the second is immediate due to Theorem 2.14)

$$\mathscr{L}^p(\Omega;\mathbb{R}^{d\times d}) \subset \mathscr{G}^p(\Omega;\mathbb{R}^{d\times d}) \subset \mathscr{P}^p(\Omega;\mathbb{R}^{d\times d}).^{22}$$

In Remark 2.12 we stated that, already from (Kružík and Roubíček, 1996), for any L^p-Young measure ν the existence of a generating sequence $\{\tilde{z}_k\}_{k=1}^\infty$ with $|z_k|^p$ weakly convergent in $L^1(\Omega)$ can be established; in particular, this holds true for any L^p-gradient Young measure. However, in order to prove Theorem 2.19 it will be important to assure that at least one such sequence consists of gradients of functions in $W^{1,p}(\Omega;\mathbb{R}^d)$. To this end, we exploit the following lemma:

Lemma 2.18. [23] *Let $p \in (1,\infty)$ and $\{z_k\}_{k=1}^\infty$ be a bounded sequence in $W^{1,p}(\Omega,\mathbb{R}^d)$ generating the gradient Young measure ν. Then there exists another bounded sequence $\{w_k\}_{k=1}^\infty \subset W^{1,p}(\Omega,\mathbb{R}^d)$ such that $\{|\nabla w_k|^p\}_{k=1}^\infty$ is weakly convergent in $L^1(\Omega)$ and the gradient Young measures associated with these sequences are same ones.*
Moreover, let z be the weak limit of the sequence $\{z_k\}_{k=1}^\infty$. Then the sequence $\{w_k\}_{k=1}^\infty$ can be chosen in such a way that $w_k - z \in W_0^{1,p}(\Omega)$ for all integers k.

With all the necessary information about Young measures at hand, let us now prove that L^p-gradient Young measures represent a correct relaxation tool for the problem (2.2).

Theorem 2.19. [24] *Let $p \in (1,\infty)$ and let the functional $I(y)$ be defined through (2.1) with ϕ continuous, satisfying the growth condition (2.3). Furthermore, let us define*

$$\bar{I}(\nu) = \int_\Omega \phi \bullet \nu \,\mathrm{d}x$$

where ϕ corresponds again to (2.1). Then

$$\inf_{y\in W^{1,p}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^d)} I(y) = \min_{\nu\in\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d})} \bar{I}(\nu).$$

[22] Note that, from (2.14) and the remarks made there, all of these inclusions are strict if $d \geq 3$

[23] This lemma was originally proved by Fonseca et al. (1998) and independently also by Kristensen (1994).

[24] This theorem can be found in e.g. (Pedregal, 1997).

Moreover, if we denoted $\{v_k\}_{k\in\mathbb{N}} \subset W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^d)$ *the infimizing sequence of* I*, a subsequence of* $\{\nabla v_k\}_{k\in\mathbb{N}}$ *generates a minimizer of* $\bar{I}$*.*

Proof. Let us choose $\{v_k\}_{k=1}^{\infty} \subset W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^d)$, an infimizing sequence of the functional $I(y)$. This sequence is, due to (2.3), bounded in $W^{1,p}_{\Gamma_D}(\Omega,\mathbb{R}^d)$; therefore gradients of a (non-relabeled) subsequence of $\{v_k\}_{k=1}^{\infty}$ generate the family of L^p-gradient Young measures denoted ν. Thus, we have, by Lemma 2.11, that

$$\int_\Omega \phi \bullet \nu \,\mathrm{d}x \le \lim_{k\to\infty} \int_\Omega \phi(\nabla v_k)\mathrm{d}x = \inf_{y\in W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^d)} I(y),$$

and consequently

$$\inf_{\bar{\nu}\in\mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^{d\times d})} \bar{I}(\bar{\nu}) \le \int_\Omega \phi \bullet \nu \,\mathrm{d}x \le \inf_{y\in W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^d)} I(y).$$

To show the equality, suppose that, by contradiction, there existed a $\tilde{\nu} \in \mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^{d\times d})$ such that $\bar{I}(\tilde{\nu}) < \bar{I}(\nu)$. Then, there had to exist a sequence $\{z_k\}_{k=1}^{\infty} \subset W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^d)$ generating $\tilde{\nu}$. Moreover due to Lemma 2.18 this sequence can be chosen in such a way that $\{\phi(\nabla z_k(x))\}_{k=1}^{\infty}$ is weakly convergent in $L^1(\Omega)$ (thanks to the assumed growth condition (2.3)) and therefore

$$\bar{I}(\nu) > \bar{I}(\tilde{\nu}) = \lim_{k\to\infty} \int_\Omega \phi(\nabla z_k)\mathrm{d}x \ge \inf_{y\in W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^d)} I(y),$$

a contradiction. □

To end this section, let us give a simple example that demonstrates how the relaxation of (2.2) by gradient Young measures can preserve useful information about infimizing sequences of the original problem.

Example 2.20. Let us choose $d = 3$ and consider $\phi : \mathbb{R}^{3\times 3} \mapsto \mathbb{R}$ in (2.2) as

$$\phi(F) = \min_{i\in\{1,2\}} (U_i^{-\mathrm{T}} F^{\mathrm{T}} F U_i^{-1} - \mathbb{I})^2, \tag{2.26}$$

where the matrices U_1, U_2 satisfy

$$U_1 - U_2 = \mathbf{a} \otimes \mathbf{n}. \tag{2.27}$$

for $\mathbf{n} = (0,0,1)$ and some vector $\mathbf{a}$. Moreover, we assume that $\frac{1}{2}U_1 + \frac{1}{2}U_2 = \mathbb{I}$. At last, let us choose $\Gamma_D = \partial\Omega$ in (2.2).

With this choice, solutions to (2.2) *do not exist*. Indeed, $I(y) \ge 0$ for all $y \in W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^d)$. Yet, since neither U_1 nor U_2 can be equal to $\mathbb{I}$ we see that $I(y) > 0$ for all $y \in W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^d)$. Still, $I(y)$ can be as near to zero as demanded by choosing y such that its gradients form a "narrow-stripe" arrangement of U_1 and U_2 like in Figure 2.1; there the gray triangles represent a transition layer in order to satisfy the boundary condition [25]. As ϕ is positive only in these gray triangles, by letting ∇y oscillate faster between U_1 and U_2 and hence reducing the measure of the gray triangles, the energy can be arbitrarily close to zero.

Therefore, the sequence of $y_k \in W^{1,2}_{\Gamma_D}(\Omega;\mathbb{R}^3)$ the gradients of which correspond to finer and finer stripes as in Figure 2.1 is an infimizing sequence of the functional I. Furthermore, (a subsequence of) $\{\nabla y_k\}$ generates the L^p-gradient Young measure $\frac{1}{2}\delta_{U_1} + \frac{1}{2}\delta_{U_2}$ which, due to Theorem 2.19, is a minimizer of the relaxed problem. This measure can, very roughly, be understood as a collection of "infinitely fine stripes" in Figure 2.1 or "infinitely fast oscillating function between U_1 and U_2".

[25] Note that, due to (2.27), y is *continuous* and hence in $W^{1,2}_{\Gamma_D}(\Omega;\mathbb{R}^3)$

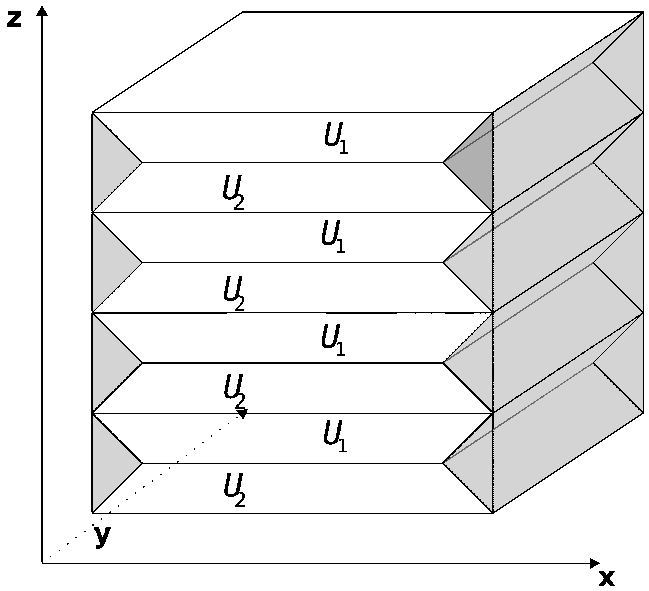


Figure 2.1: Infimizing sequence of (2.2) with ϕ from (2.26).

2.3.2 (Gradient) Young measures generated by invertible sequences

So far, when qualifying ϕ in (2.1), we demanded the continuous function ϕ to *satisfy* (2.3). However, if the minimization problem in (2.2) should represent the search for stable states in *elasticity* (with ∇y being then the *deformation gradient*) one should also require that

$$\phi(A) \to +\infty \text{ whenever } \det A \to 0_+. \tag{2.28}$$

Note, that this is in *contradiction* to (2.3).

One possibility to assure (2.28), is to generalize the preceding theory by letting ϕ depend also on A^{-1} and extending (2.3) as

$$c(-1 + |A|^p + |A^{-1}|^p) \le \phi(A) \le \tilde{c}(1 + |A|^p + |A^{-1}|^p).$$

Physically, this introduces just another strain measure from the Seth-Hill family of strain measures (Curnier and Rakotomanana, 1991; Šilhavý, 1997).

This motivates the study of Young measures generated by a.e. on Ω invertible matrices bounded together with its inverse in $L^p(\Omega;\mathbb{R}^{d\times d})$. Such measures have recently been characterized by Benešová, Kružík and Pathó (2012). In this paper, measures generated by a.e. on Ω invertible gradients of maps in $W^{1,\infty}(\Omega;\mathbb{R}^d)$ with an essentially bounded inverse were considered, too.

Though we cannot use these results for relaxation in shape-memory alloys later in Chapters 4 and 5, since, in this setting, equivalents of Theorem 2.14 and Lemma 2.18 are still missing, we will give the main results of (Benešová, Kružík and Pathó, 2012) together with the most important proof ingredients because of their independent interest.

Note that, because the support of the resulting parameterized measures is of particular importance in this section, we avoid to use the shortening "$\bullet$" for the momentum operator within it.

Let us first introduce the subset of L^p-Young measures

$$\mathscr{Y}^{p,-p}(\Omega;\mathbb{R}^{d\times d}) := \Big\{\nu\in\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d});\ \int_\Omega\int_{\mathbb{R}^{d\times d}_{\rm inv}}(|s|^p+|s^{-1}|^p)\nu_x(\mathrm{d}s)\,\mathrm{d}x<+\infty\ ,\\ \nu_x(\mathbb{R}^{d\times d}_{\rm inv})=1 \text{ for a.a. } x\in\Omega\Big\}; \tag{2.29}$$

recall that $\mathbb{R}^{d\times d}_{\rm inv}$ denotes the set of *invertible* matrices.

Then, this subset of L^p-Young measures can be generated by bounded sequences of matrices in $L^p(\Omega;\mathbb{R}^{d\times d})$ that are a.e. invertible with their inverse also bounded in $L^p(\Omega;\mathbb{R}^{d\times d})$; this is summarized in the following theorem:

Theorem 2.21. *Let $p\in(1,\infty)$, and let $\{Y_k\}_{k\in\mathbb{N}}$, $\{Y_k^{-1}\}_{k\in\mathbb{N}}\subset L^p(\Omega;\mathbb{R}^{d\times d})$ be bounded. Then there is a subsequence of $\{Y_k\}_{k\in\mathbb{N}}$ (not relabeled) and $\nu\in\mathscr{Y}^{p,-p}(\Omega;\mathbb{R}^{d\times d})$ such that for every $g\in L^\infty(\Omega)$ and every $v\in C_{p,-p}(\mathbb{R}^{d\times d}_{\rm inv})$[26] it holds that*

$$\lim_{k\to\infty}\int_\Omega v(Y_k(x))g(x)\,\mathrm{d}x=\int_\Omega\int_{\mathbb{R}^{d\times d}_{\rm inv}}v(s)\nu_x(\mathrm{d}s)g(x)\,\mathrm{d}x\ , \tag{2.30}$$

Conversely, if $\nu\in\mathscr{Y}^{p,-p}(\Omega;\mathbb{R}^{d\times d})$ then there exists bounded sequence $\{Y_k\}_{k\in\mathbb{N}}\subset L^p(\Omega;\mathbb{R}^{d\times d})$ such that $\{Y_k^{-1}\}_{k\in\mathbb{N}}\subset L^p(\Omega;\mathbb{R}^{d\times d})$ is also bounded and (2.30) holds for all g and v defined above.

The proof Theorem 2.21 can be established very similarly as in (Kružík and Roubíček, 1996) or (Pedregal, 1997); however, an *important additional ingredient for the necessary condition* is to establish that any Young measure generated by a sequence $\{Y_k\}_{k\in\mathbb{N}}$ that is bounded together with its inverse in $L^p(\Omega;\mathbb{R}^{d\times d})$ is supported on invertible matrices $\mathbb{R}^{d\times d}_{\rm inv}$. This is assured by the following proposition:

Proposition 2.22. [27] *Let $\{Y_k\}_{k\in\mathbb{N}}\subset L^p(\Omega;\mathbb{R}^{d\times d})$ generate $\nu\in\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d})$ and let $\int_\Omega|\mathrm{det}Y_k^{-1}|^q\,\mathrm{d}x\le C$ for some $C>0$ and some $q>0$. Then for almost all $x\in\Omega$ ν_x is supported on $\mathbb{R}^{d\times d}_{\rm inv}$ in the sense that $\nu_x(\mathbb{R}^{d\times d}\setminus\mathbb{R}^{d\times d}_{\rm inv})=0$ for almost all $x\in\Omega$.*

Proof. Assume that the assertion did not hold, i.e., that there existed a measurable $\omega\subset\Omega$ with positive measure such that $\int_\omega\int_{\mathbb{R}^{d\times d}\setminus\mathbb{R}^{d\times d}_{\rm inv}}\nu_x(\mathrm{d}s)\,\mathrm{d}x>0$. Then, for any $\epsilon>0$, define a smooth cut-off $\Phi^{\det,0}_\epsilon$ such that $\Phi^{\det,0}_\epsilon(s)=1$ on $\mathbb{R}^{d\times d}\setminus\mathbb{R}^{d\times d}_{\rm inv}$ and $\Phi^{\det,0}_\epsilon(s)=0$ for all $s\in\mathbb{R}^{d\times d}_{\rm inv}$ such that $|\det s|\ge\epsilon$.[28] We have by Lemma 2.11

$$\lim_{k\to\infty}\int_\omega\Phi^{\det,0}_\epsilon(Y_k(x))\,\mathrm{d}x=\int_\omega\int_{\mathbb{R}^{d\times d}}\Phi^{\det,0}_\epsilon(s)\nu_x(\mathrm{d}s)\,\mathrm{d}x\ge\int_\omega\int_{\mathbb{R}^{d\times d}\setminus\mathbb{R}^{d\times d}_{\rm inv}}\nu_x(\mathrm{d}s)\,\mathrm{d}x=:\delta>0\ . \tag{2.31}$$

Hence, there is $k_0\in\mathbb{N}$ such that $\int_\omega\Phi^{\det,0}_\epsilon(Y_k(x))\,\mathrm{d}x>\delta/2$ if $k>k_0$; i.e. if the assertion was false there always exists a measurable set denoted $\omega(k)\subset\Omega$, $|\omega(k)|>\delta/2$ such that $|\det\,Y_k(x)|^q<\varepsilon^q$ if $x\in\omega(k)$. Consequently, $|\det\,Y_k^{-1}(x)|^q>\varepsilon^{-q}$ if $x\in\omega(k)$. Thus, for every $k>k_0$

$$\int_\Omega|\det\,Y_k^{-1}(x)|^q\,\mathrm{d}x\ge\int_{\omega(k)}|\det\,Y_k^{-1}(x)|^q\,\mathrm{d}x\ge\frac{\delta}{2\varepsilon^q}\ . \tag{2.32}$$

As $\varepsilon>0$ is arbitrary it contradicts the bound $\int_\Omega|\mathrm{det}Y_k^{-1}|^q\,\mathrm{d}x\le C$. □

[26] $C_{p,-p}(\mathbb{R}^{d\times d}_{\rm inv})$ was defined in (2.4).

[27] Taken from (Benešová, Kružík and Pathó, 2012).

[28] $\Phi^{\det,0}_\epsilon$ can be found as follows: first of all find a smooth $\varphi_\epsilon:\mathbb{R}\to\mathbb{R}$ such that $\varphi_\epsilon(0)=1$ and $\varphi_\epsilon(x)=0$ for $|x|>\epsilon$. Then define $\Phi^{\det,0}_\epsilon(s)=\varphi_\epsilon(\det s)$.

Having obtained a characterization of Young measures generated (roughly) by invertible bounded matrices with a bounded inverse, we would like to establish a similar characterization also for the gradient case. Within the work on this thesis, only results in the L^∞-case have been obtained (cf. (Benešová, Kružík and Pathó, 2012)); they are summarized below.

Let us first introduce the set of *gradient Young measures supported on invertible matrices* $\mathscr{G}^{+\infty,-\infty}(\Omega;\mathbb{R}^{d\times d})$ by the following construction: we define

$$\mathscr{G}^{+\infty,-\infty}_{\varrho}(\Omega;\mathbb{R}^{d\times d}) := \Big\{\nu\in\mathscr{Y}^{\infty}(\Omega;\mathbb{R}^{d\times d});\ \exists\{y_k\}\subset W^{1,\infty}(\Omega;\mathbb{R}^d)\ ,\\ \text{for a.a. } x\in\Omega\ \{\nabla y_k(x)\}\subset R^{d\times d}_{\varrho} \text{ and } \{\nabla y_k\}_{k\in\mathbb{N}} \text{ generates } \nu\Big\}$$

with $R^{d\times d}_{\varrho} := \{A\in\mathbb{R}^{d\times d}_{\mathrm{inv}};\ \max(|A|,|A^{-1}|)\le\varrho\}$; then

$$\mathscr{G}^{+\infty,-\infty}(\Omega;\mathbb{R}^{d\times d}) := \cup_{\varrho>0}\mathscr{G}^{+\infty,-\infty}_{\varrho}(\Omega;\mathbb{R}^{d\times d}). \tag{2.33}$$

The set $\mathscr{G}^{+\infty,-\infty}(\Omega;\mathbb{R}^{d\times d})$ can be characterized similarly as the set of gradient Young measures in Theorem 2.13; however we need to introduce a different an additional condition on the support of the measure and a generalization of the quasiconvex envelope (introduced below) has to be used.

First, we specify the set of admissible test functions; to this end, put $R^{d\times d}_{+\infty} := \mathbb{R}^{d\times d}_{\mathrm{inv}}$ and denote for $\varrho\in(0;+\infty]$

$$\mathscr{O}(\varrho) := \{v:\mathbb{R}^{d\times d}\to\mathbb{R}\cup\{+\infty\};\ v\in C(R^{d\times d}_{\varrho})\ ,\ v(s)=+\infty \text{ if } s\in\mathbb{R}^{d\times d}\setminus R^{d\times d}_{\varrho}\}\ .$$

If $F\in\mathbb{R}^{d\times d}$ and $v\in\mathscr{O}(\varrho)$ we denote by $Q_{\mathrm{inv}}v:\mathbb{R}^{d\times d}\to\mathbb{R}\cup\{+\infty\}$ the function

$$Q_{\mathrm{inv}}v(F) := \frac{1}{|\Omega|}\inf_{y\in\mathscr{U}_F}\int_\Omega v(\nabla y(x))\,\mathrm{d}x\ , \tag{2.34}$$

where

$$\mathscr{U}_F := \{y\in W^{1,\infty}(\Omega;\mathbb{R}^d);(\nabla y)^{-1}\in L^\infty(\Omega;\mathbb{R}^{d\times d}),\quad y(x)=Fx \text{ for } x\in\partial\Omega\}\ . \tag{2.35}$$

Remark 2.23. Note that (2.34) also introduced a "variation of quasiconvexity". Indeed, we could say that $\varphi:\mathbb{R}^{d\times d}_{\mathrm{inv}}\to\mathbb{R}$ is $Q_{\mathrm{inv}}-$convex if $Q_{\mathrm{inv}}\varphi(F)=\varphi(F)$ for all $F\in\mathbb{R}^{d\times d}$. Clearly, any $W^{1,p}-$*quasiconvex* function is also $Q_{\mathrm{inv}}-$convex; however, the opposite does not need to be true. To see this, consider just the function $\phi:\mathbb{R}\to\mathbb{R}$ (depicted in Figure 2.23) such that $\phi(0)=0$ and $\phi(x)=1$ for all $x\neq 0$. Then this ϕ is not *convex* (*not quasiconvex*) but it is $Q_{\mathrm{inv}}-$convex.

Theorem 2.24. [29] *Let $\nu\in\mathscr{Y}^{\infty}(\Omega;\mathbb{R}^{d\times d})$. Then $\nu\in\mathscr{G}^{+\infty,-\infty}(\Omega;\mathbb{R}^{d\times d})$ if and only if the following three conditions hold*

1. $\operatorname{supp}\nu_x\subset R^{d\times d}_{\varrho}$ *for a.a.* $x\in\Omega$ *and some* $\varrho>0$,
2. $\exists\ u\in W^{1,\infty}(\Omega;\mathbb{R}^d)\ :\ \nabla u(x)=\int_{\mathbb{R}^{d\times d}_{\mathrm{inv}}} s\,\nu_x(\mathrm{d}s)$ *for a.a.* $x\in\Omega$,
3. *for a.a.* $x\in\Omega$ *all* $\tilde\varrho\in(\varrho;+\infty]$, *and all* $v\in\mathscr{O}(\tilde\varrho)$ *the following inequality is valid*

$$Q_{\mathrm{inv}}v(\nabla u(x))\le\int_{\mathbb{R}^{d\times d}_{\mathrm{inv}}} v(s)\nu_x(\mathrm{d}s)\ .$$

[29] Taken from (Benešová, Kružík and Pathó, 2012).

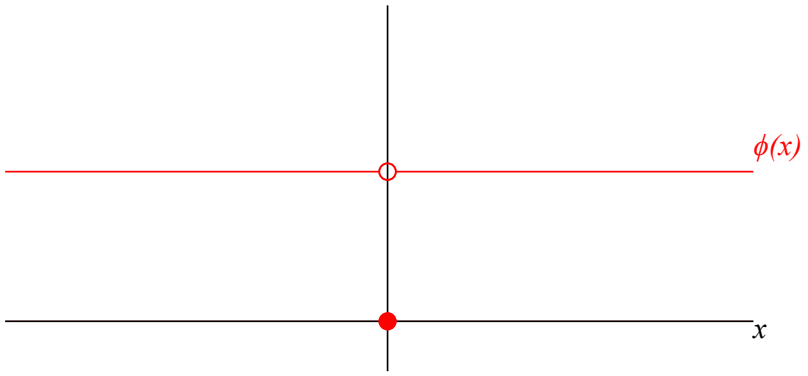


Figure 2.2: An example of a function that is $Q_{\text{inv}}-$convex, however not convex.

This theorem can be proved similarly as Theorem 2.13, the proof which can be found e.g. in (Kinderlehrer and Pedregal, 1994; Pedregal, 1997); however, one has to be careful when in comes to the use of cut-off techniques. Indeed the proof in (Kinderlehrer and Pedregal, 1994; Pedregal, 1997) relies in several places on the fact that for any gradient Young measure a generated sequence can be found, all elements of which have the same boundary value as the weak* limit of the sequence. To prove this fact, a cut-off technique is used in (Pedregal, 1997).

To obtain a similar result also in this case, clearly, the conventional cut-off technique is not suitable since we cannot guarantee that, after a cut-off has been used, the resulting gradients in the sequence are still invertible. To circumpass this problem, we can rely Lemma 2.25.

First, let us recall that $O(d)$ id the set of orthogonal matrices in $\mathbb{R}^{d\times d}$ and denote by $\lambda_d(A)$ the largest singular value of $A \in \mathbb{R}^{d\times d}$, i.e., the largest eigenvalue of $\sqrt{A^\top A}$.

Lemma 2.25. [30] *Let $\omega \subset \mathbb{R}^d$ be open and Lipschitz. Let $\varphi \in W^{1,\infty}(\omega;\mathbb{R}^d)$ be such that there is $\vartheta > 0$, so that $0 \le \lambda_d(\nabla\varphi) \le 1-\vartheta$ a.e. in ω. Then, there exist mappings $u \in W^{1,\infty}(\omega;\mathbb{R}^d)$ for which $\nabla u \in O(d)$ a.e. in ω and $u = \varphi$ on $\partial\omega$. Moreover, the set of such mappings is dense (in the L^∞ norm) in the set $\{\psi := z+\varphi;\ z \in W_0^{1,\infty}(\omega;\mathbb{R}^d)\ ,\ \lambda_d(\nabla\psi) \le 1-\vartheta$ a.e. in $\omega\}$.*

With the aid of this lemma, we are now able to prove the following Proposition 2.26; this Proposition, in turn, allows us to follow the arguments of (Pedregal, 1997) to prove Theorem 2.24.

Proposition 2.26. *Let $F \in \mathbb{R}^{d\times d}$, $u_F(x) := Fx$, $y_k \overset{*}{\rightharpoonup} u_F$ in $W^{1,\infty}(\Omega;\mathbb{R}^d)$ and let, for some $\alpha > 0$, $\nabla y_k(x) \in R^{d\times d}_\alpha$ for all $k > 0$ and almost all $x \in \Omega$. Then for every $\varepsilon > 0$ there is a sequence $\{u_k\} \subset W^{1,\infty}(\Omega;\mathbb{R}^d)$ such that $\nabla u_k(x) \in R^{d\times d}_{\alpha+\varepsilon}$ for all $k > 0$ and almost all $x \in \Omega$, $u_k - u_F \in W_0^{1,\infty}(\Omega;\mathbb{R}^d)$ and $|\nabla y_k - \nabla u_k| \to 0$ in measure. In particular, $\{\nabla y_k\}$ and $\{\nabla u_k\}$ generate the same Young measure.*

Proof. Define for $\ell > 0$ sufficiently large $\Omega_\ell := \{x \in \Omega;\ \operatorname{dist}(x,\partial\Omega) \ge 1/\ell\}$ and the smooth cut-off functions $\eta_\ell : \Omega \to [0,1]$

$$\eta_\ell(x) = \begin{cases} 1 & \text{if } x \in \Omega_\ell \\ 0 & \text{if } x \in \partial\Omega \end{cases}$$

such that $|\nabla\eta_\ell| \le C\ell$ for some $C > 0$. Define $z_{k\ell} := \eta_\ell y_k + (1-\eta_\ell)u_F$. Then $z_{k\ell} \in W^{1,\infty}(\Omega;\mathbb{R}^d)$ and $z_{k\ell} = y_k$ in Ω_ℓ and $z_{k\ell} = u_F$ on $\partial\Omega$. We see that $\nabla z_{k\ell} = \eta_\ell\nabla y_k + (1-$

[30] This can be found in (Dacorogna and Marcellini, 1999, p. 199 and Remark 2.4).

$\eta_\ell)F+(y_k-u_F)\otimes\nabla\eta_\ell$. Hence, in view of the facts that $|F| \le \liminf_{k\to\infty} \|\nabla y_k\|_{L^\infty(\Omega;\mathbb{R}^{d\times d})} \le \alpha$ and that $y_k \to u_F$ uniformly in $\bar\Omega$, we can extract for every $\varepsilon > 0$ a subsequence $k = k(\ell)$ such that

$$\|\nabla z_{k(\ell)\ell}\|_{L^\infty(\Omega;\mathbb{R}^{d\times d})} < \alpha + \frac{\varepsilon}{2}\,.$$

Consequently, $\{z_{k(\ell)\ell}\}$ is uniformly bounded in $W^{1,\infty}(\Omega;\mathbb{R}^d)$. Moreover,

$$\lambda_n\left(\frac{\nabla z_{k(\ell)\ell}}{\alpha+\varepsilon}\right) \le \frac{\|\nabla z_{k(\ell)\ell}\|_{L^\infty}}{\alpha+\varepsilon} \le 1 - \frac{\varepsilon}{2(\alpha+\varepsilon)}\,,$$

where we used the inequality $\lambda_d(A) \le |A|$ for any $A \in \mathbb{R}^{d\times d}$. Denote $\omega_\ell = \Omega \setminus \Omega_\ell$. Then $w_{k(\ell)\ell} = z_{k(\ell)\ell}|_{\omega_\ell}/(\alpha+\varepsilon)$ is such that $\lambda_n(\nabla w_{k(\ell)\ell}) \le 1-\vartheta$ for $\vartheta := \varepsilon/2(\alpha+\varepsilon)$. We use Lemma 2.25 for $\omega := \omega_\ell$ and $\varphi := w_{k(\ell)\ell}$ to obtain $\phi_{k(\ell)\ell} \in W^{1,\infty}(\omega_\ell;\mathbb{R}^n)$ such that $\phi_{k(\ell)\ell} = w_{k(\ell)\ell}$ on $\partial\omega_\ell$ and $\nabla\phi_{k(\ell)\ell} \in O(n)$. Define

$$u_{k(\ell)\ell} = \begin{cases} y_k & \text{if } x \in \Omega_\ell \\ (\alpha+\varepsilon)\phi_{k(\ell)\ell} & \text{if } x \in \Omega\setminus\Omega_\ell. \end{cases}$$

Notice that $\{u_{k(\ell)\ell}\}_{\ell\in\mathbb{N}} \subset W^{1,\infty}(\Omega;\mathbb{R}^d)$ and that $u_{k(\ell)\ell}(x) = Fx$ for $x \in \partial\Omega$. Further, $\nabla u_{k(\ell)\ell} \in R^{d\times d}_{\alpha+\varepsilon}$. Moreover, $\nabla u_{k(\ell)\ell} \ne \nabla y_k$ only on sets of vanishing measure, therefore they generate the same Young measure by (Pedregal, 1997, Lemma 8.3). □

Chapter 3

Framework of generalized standard solids

Let us introduce the so-called *framework of generalized standard materials* suited for *description of dissipative processes in solids*; we shall exploit this concept in Chapters 4 and 5. The main assumption of this concept is that (apart from the heat flux) only two functions, namely the *free energy* and a *dissipation potential*[1] need to be chosen constitutively. A large number of rheological models falls into this framework, as e.g. the standard *Maxwell* or *Kelvin* model.

In this introductory chapter, we largely follow the book of Nguyen (2000), who together with Halphen introduced this framework in 1975 (Halphen and Nguyen, 1975); let us just note, however, that even before the notion of a "flow potential" was used by Rice (1971) to substitute the concept of yield surfaces used in plasticity. Since then, the framework of generalized standard solids has been widely used in modeling of e.g. plasticity, delamination, damage, crack propagation or phase transitions (a not exhaustive list includes (Arndt et al., 2006; Bartel and Hackl, 2008, 2009; Frost et al., 2010; Knees and Mielke, 2010; Maugin, 1992; Mielke et al., 2009, 2010; Roubíček et al., 2009; Sadjadpour and Bhattacharya, 2007*b*; Toader and Zanini, 2009)) and has been further analyzed from thermodynamical (e.g.(Hackl and Fischer, 2008; Houlsby and Puzrin, 2000)) and mathematical (e.g. (Francfort and Mielke, 2006; Mainik and Mielke, 2005; Mielke, 2003, 2005)) point of view; note that an independent but closely related concept was developed by Petryk (2003).

Let us stress that, in the physical derivations in this chapter, all functions are assumed *sufficiently smooth*. If the smoothness is not given, balance equations would be satisfied only in an appropriate weak setting.

3.1 Continuum thermodynamics in a nutshell

In order to introduce the framework, let us review some basic concepts from continuum thermodynamics within this section.

A basic assumption of continuum thermodynamics (cf. e.g. (Nguyen, 2000)) is that "*the (continuum mechanical) system is composed of infinitesimal sub-systems in slow evolution such that each sub-system can be always considered as almost in thermodynamic equilibrium at any time*"; a material point is then supposed to be composed of one of these infitesimal sub-systems. Of course, the system as whole does not have to be in equilibrium anymore. Still, this *local state postulate* allows us to introduce locally

[1] The name dissipation potential is sometimes disputed and instead the name *dissipation function* (e.g. (Petryk, 2003)) is used. We shall give more details on this in Subsection 3.2.

the *entropy* and thermodynamic potentials (like the *internal energy* or the *Helmholtz or Gibbs free energy*)[2] as functions of so-called *state variables*. Those are variables that characterize the current state of the system. One of these variables is, clearly, the temperature θ, another obvious choice is some measure of deformation $\mathbb{Y}$; this can be e.g. the deformation $y : \Omega \to \mathbb{R}^d$ itself or the deformation gradient ∇y. Shall other state variables be necessary, they will be denoted simply by χ.[3].

Hence, one can introduce the *entropy* $s = s(\theta, \mathbb{Y}, \chi)$ and the internal energy $e = e(\theta, \mathbb{Y}, \chi)$.[4]

The **first law of thermodynamics**, which states that the overall energy in a closed system has to be conserved, is then expressed in form of the following balance: (cf. e.g. (Gurtin et al., 2010; Nguyen, 2000))[5]

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\underbrace{\int_V \frac{\rho}{2}|\dot{y}|^2 \,\mathrm{d}x}_{\text{kinetic energy}} + \underbrace{\int_V \rho e(\theta, y, \chi)\,\mathrm{d}x}_{\text{internal energy}} \Big) = \underbrace{\int_V f\cdot\dot{y}\,\mathrm{d}x + \int_{\partial V}(\mathcal{P}n)\cdot\dot{y}\,\mathrm{d}S}_{\text{external power}} - \underbrace{\int_{\partial V} q\cdot n\,\mathrm{d}S}_{\text{heat flow}} \tag{3.1}$$

for any control volume $V \subset \Omega$. Here f is the applied body force and $\mathcal{P}$ is the first Piola-Kirchhoff stress tensor (so that $\mathcal{P}n$ represents the surface force on the boundary of V), q is the heat flux, ρ is the density of the specimen and n is the outer normal to ∂V.

Further, we exploit also the well-known balance of momentum equations (here written in local form with boundary conditions omitted)

$$\mathrm{div}\mathcal{P} + f = \rho\ddot{y} \qquad \forall x \in \Omega, \tag{3.2}$$

when multiplying it by $\dot{y}$ and integrating over V; this gives

$$\int_V (\mathrm{div}\mathcal{P})\cdot\dot{y}\,\mathrm{d}x + \int_V f\cdot v\,\mathrm{d}x = \int_V \rho\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\dot{y}|^2\,\mathrm{d}x,$$

which, after applying the divergence theorem (see e.g. (Gurtin et al., 2010, page 312)) yields

$$\int_{\partial V}(\mathcal{P}n)\cdot\dot{y}\,\mathrm{d}x - \int_V \mathcal{P} : \nabla\dot{y} + \int_V f\cdot v\,\mathrm{d}x = \int_V \rho\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\dot{y}|^2\,\mathrm{d}x; \tag{3.3}$$

this expression is sometimes referred to as the *balance of mechanic energy*. Combining this equation with (3.1), exploiting ones again the divergence theorem and assuming (naturally for solids) that the density ρ *does not depend on time* finally gives the following global form of the first law of thermodynamics:

$$\int_V \dot{e}(\theta, \mathbb{Y}, \chi)\,\mathrm{d}x = \int_V \mathcal{P} : \nabla\dot{y} - \mathrm{div}(q)\,\mathrm{d}x. \tag{3.4}$$

Since the control volume V was arbitrary, (3.4) yields[6] the following local form

$$\rho\dot{e}(\theta, y, \chi) = \mathcal{P} : \nabla\dot{y} - \mathrm{div}(q). \tag{3.5}$$

[2]Note that, since these quantities are *only* defined in equilibrium (cf. e.g. (Callen, 1985)), it would not be possible to define these principal thermodynamic functions without this postulate.

[3]The state variables depend, of course, on time t and the position x of the material point in reference domain Ω.

[4]Usually in thermodynamics, the internal energy is understood to depend on the entropy rather then on temperature, see (Callen, 1985). Later, we shall, however, work with a Legendre-Fenchel transform of the internal energy (which forms the so-called *free energy*) which depends on the temperature indeed.

[5]For simplicity we assume zero external heat sources, like radiation. Also note that we work in the Lagragean description here while, mostly, balance laws are formulated in the Euler's description.

[6]Sufficient smoothness is assumed to be granted, as elsewhere in this section.

The **second law of thermodynamics** can be expressed as follows: *given any control volume $V \subset \Omega$, the increase of the entropy in this volume must be non-negative.* When realizing that the total entropy can be increased, besides by its production in the volume, also by transporting heat to the volume through the boundary, this statement can be formalized as

$$\text{Entropy increase} = \int_V \rho\dot{s}\,\mathrm{d}x + \int_{\partial V} \frac{q}{\theta}\cdot n\,\mathrm{d}S \geq 0. \tag{3.6}$$

Exploiting once again the divergence theorem, this can be reformulated as

$$\int_V \rho\dot{s} + \operatorname{div}\left(\frac{q}{\theta}\right)\mathrm{d}x \geq 0,$$

which allows us (as the control volume V is arbitrary) to deduce the following local form of the second law of thermodynamics

$$\rho\dot{s} - \operatorname{div}\left(\frac{q}{\theta}\right) \geq 0.$$

It shall be more advantageous, for our purposes, to reformulate this equation by combining it with the already obtained local form of the first law of thermodynamics (3.5) to obtain an equivalent form of the second law, that is sometimes referred to as the *Clausius-Duhem inequality*, [7]

$$\theta\rho\dot{s} - \rho\dot{e} + \mathcal{P} : \nabla\dot{y} - \frac{q\cdot\nabla\theta}{\theta} \geq 0.$$

Since we will work rather with free energies (and prescribe them constitutively) than with the internal energy, we introduce the Helmholtz free energy ψ as

$$\psi = e - \theta s. \tag{3.7}$$

This allows us to reformulate the second law of thermodynamics into its most suitable form for our purposes as follows:

$$\mathscr{D} = \mathcal{P} : \nabla\dot{y} - \rho\dot{\psi} - \rho s\dot{\theta} - \frac{q\cdot\nabla\theta}{\theta} \geq 0. \tag{3.8}$$

where $\mathscr{D}$ is referred to as *dissipation* or sometimes, more exactly, *rate of dissipation.*

3.1.1 Example: Reversible processes in solids

We shall understand those processes that produce *zero dissipation* as *reversible processes.* For these processes we, hence, have

$$\mathcal{P} : \nabla\dot{y} - \rho\dot{\psi} - \rho s\dot{\theta} - \frac{q\cdot\nabla\theta}{\theta} = 0$$

Recall that we assumed $\psi = \psi(\theta, \mathbb{Y}, \chi)$ with $\mathbb{Y}$ some measure of deformation. For the sake of clarity, let us assume the concept of so-called *simple materials* when $\mathbb{Y} = \nabla y$[8]. Then the zero-dissipation requirement leads to

$$(\mathcal{P} - \rho\psi'_{\nabla y}) : \nabla\dot{y} + \rho(-s - \psi'_\theta)\dot{\theta} - \rho\psi'_\chi\dot{\chi} - \frac{q\cdot\nabla\theta}{\theta} = 0.$$

[7] We need to rewrite $\operatorname{div}\left(\frac{q}{\theta}\right) = \frac{\operatorname{div} q}{\theta} - \frac{q\cdot\nabla\theta}{\theta^2}$, multiply the local form of the second law of thermodynamics by θ and finally subtract (3.5).

[8] Note that if the choice of variables had to be more complicated, e.g. if $\mathbb{Y} = (y, \nabla y)$, we could, for the calculations in this section, include y in the set of the remaining state variables χ.

Since the change of all state variables is considered *independent* this equation can be satisfied if only if

$$s = -\psi'_\theta(\theta, \nabla y), \tag{3.9}$$
$$\mathcal{P} = \rho\psi'_{\nabla y}(\theta, \nabla y), \tag{3.10}$$
$$q = 0, \tag{3.11}$$

and the Helmholtz free energy depends *only* on θ, ∇y and no other variable.

Note that (3.9) is known as the *Gibbs relation* and (3.10) yields the response of a *hyperelastic* material.

3.1.2 Irreversible processes in solids

Let us now turn our attention to irreversible processes characterized by an *overall positive* dissipation. While for reversible processes there is a general agreement to use the framework of entropy maximization or, equivalently, minimization of an appropriate (free) energy, the situation is much less well understood in this case (Callen, 1985).

Here, we follow the approach of (Nguyen, 2000), that will be suitable for our modeling purposes, which is in correspondence with an often used approach of fluxes and generalized forces as presented e.g. in (Callen, 1985).

First, let us distinguish between thermal and mechanic dissipation when defining

$$\mathscr{D}_{\text{mech}} = \mathcal{P} : \nabla\dot{y} - \rho\dot{\psi} + \rho s\dot{\theta}, \tag{3.12}$$
$$\mathscr{D}_{\text{therm}} = -\frac{q\cdot\nabla\theta}{\theta}. \tag{3.13}$$

Following (Nguyen, 2000), we assume that thermal and mechanic processes are independent in the sense that both, thermal and the mechanic dissipation, need to be non-negative.[9]

Throughout this thesis, we shall limit our attention only to processes in which the heat flux is governed by the Fourier law

$$q = -\mathbb{K}(\theta, \mathbb{Y}, \chi)\nabla\theta, \tag{3.14}$$

and hence thermal dissipation shall be non-negative if $\mathbb{K}$ is *positive definite* (with θ assumed non-negative, of course).

Let us, therefore, focus on mechanic dissipation. Again let us assume that $\mathbb{Y} = \nabla y$ when "hiding" possible necessary generalizations to the variable χ. Furthermore, let us allow for $\mathcal{P}$ *to depend beside the state variables themselves also on their rates*,[10] because these characterize the evolution towards equilibrium and hence seem to be of importance. Still, let us introduce the following split

$$\mathcal{P}(\theta, \dot{\theta}, \nabla y, \nabla\dot{y}, \chi, \dot{\chi}) = \mathcal{P}_{\text{el}}(\theta, \nabla y, \chi) + \mathcal{P}_{\text{in}}(\theta, \dot{\theta}, \nabla y, \nabla\dot{y}, \chi, \dot{\chi}),$$

such that $\mathcal{P}_{\text{in}}(\theta, \dot{\theta}, \nabla y, \nabla\dot{y}, \chi, \dot{\chi}) = 0$ if $(\dot{\theta}, \nabla\dot{y}, \dot{\chi}) = 0$. So, $\mathcal{P}_{\text{el}}$ is the part of the Piola-Kirchhoff tensor present in equilibrium while $\mathcal{P}_{\text{in}}$ accounts for inelastic processes. Then,

[9] Even if one could not be certain that mechanic and thermal dissipation is caused by *independent* processes, requiring that $\mathscr{D}_{\text{mech}} \geq 0$ and $\mathscr{D}_{\text{therm}}$ is always *sufficient* in order to satisfy the second law of thermodynamics. Thus, if in our modeling approach we pose this assumption we might exclude some very sophisticated, even though thermodynamically consistent, models but can always *easily verify* that the proposed model is indeed in accordance with the laws of thermodynamics.

[10] Note that we do not allow this for thermodynamic potentials ψ and s since they are *only* defined in equilibrium of every material point and hence have to depend on the state variables only.

the mechanic dissipation inequality reads as

$$\Big(\big(\mathcal{P}_{\text{el}}(\theta, \nabla y, \chi) - \rho\psi'_{\nabla y}(\theta, \nabla y, \chi)\big) : \nabla\dot{y} + \rho\big(\psi'_\theta(\theta, \nabla y, \chi) + s\big)\dot{\theta} \\ - \rho\psi'_\chi(\theta, \nabla y, \chi)\dot{\chi} + \mathcal{P}_{\text{in}}(\theta, \dot{\theta}, \nabla y, \nabla\dot{y}, \chi, \dot{\chi}) : \nabla\dot{y} \Big) \geq 0$$

Following the classical Coleman-Noll procedure (Coleman and Noll, 1963) one gets that the second law of thermodynamics is satisfied *if and only if*[11]

$$\begin{aligned} \mathcal{P}_{\text{el}}(\theta, \nabla y, \chi) &= \rho\psi'_{\nabla y}(\theta, \nabla y, \chi) \\ s &= -\psi'_\theta(\theta, \nabla y, \chi) \\ -\rho\psi'_\chi(\theta, \nabla y, \chi)\dot{\chi} + \mathcal{P}_{\text{in}}(\theta, \dot{\theta}, \nabla y, \nabla\dot{y}, \chi, \dot{\chi}) : \nabla\dot{y} &\geq 0, \end{aligned}$$

with the last expression referred to as the *reduced dissipation inequality*.

Consistently with the common approach of irreversible thermodynamics of generalized forces and fluxes (Callen, 1985), we would call $-\psi'_\chi$ (and also $\mathcal{P}_{\text{in}}$ as in (Nguyen, 2000)) the *generalized forces* and $\dot{\chi}$ (and also $\nabla\dot{y}$) the *generalized fluxes*. This nomenclature follows from the idea that if $\mathcal{P}_{\text{in}}$ and ψ'_χ are non-zero[12] the system cannot be in equilibrium because the mechanical dissipation is positive. So, the system tries to reach equilibrium through an irreversible process and forces ∇y and χ to change in order to do so. Hence, $\mathcal{P}_{\text{in}}$ and ψ_χ' "enforces" a flux $(\nabla\dot{y}, \dot{\chi})$ towards equilibrium.

If we shortly denote $A = (\mathcal{P}_{\text{in}}, -\rho\psi'_\chi)$ the vector of generalized forces and $\dot{\alpha} = (\dot{\nabla y}, \dot{\chi})$ the vector of generalized fluxes, the reduced dissipation inequality can be written compactly as

$$A{\cdot}\dot{\alpha} \geq 0.$$

Since we are considering irreversible processes here, they *cannot be fully determined by those constitutive quantities that determine reversible processes*, therefore a constitutive relation between the generalized forces and fluxes has to be prescribed, i.e.

$$\dot{\alpha} = \mathcal{T}(A, \alpha), \tag{3.15}$$

where $\mathcal{T}$ needs not to be a function, but can be an operator so that $\dot{\alpha}$ can, for example, be a solution of a differential equation or even a more complicated procedure. Choosing $\mathcal{T}$ constitutively then specifies the dissipative mechanism present in the solid; however, $\mathcal{T}$ cannot be chosen arbitrarily since we are restricted by the second law of thermodynamics. A convenient procedure to prescribe $\mathcal{T}$ that respects this law is shown in the next section.

3.2 Description of a generalized standard material by two potentials

A widely used concept on how to prescribe (3.15) is by choosing a so-called *dissipation potential* R such that

$$A \in \partial_{\dot{\alpha}} R(\alpha, \dot{\alpha}), \tag{3.16}$$

[11] While the sufficiency is easy to see, the necessity is usually proved by claiming that always a process can be constructed such that rates of the state variables are independent. In easy cases an explicit construction can be found in e.g. (Callen, 1985); however, constructing these processes in e.g. the situation here can be very difficult. Anyhow, our main concern is to deduce *sufficiency conditions* to develop thermodynamically consistent models.

[12] It is assumed that the fluxes cannot be zero, if the generalized forces are non-zero (Callen, 1985).

where ∂ is the sub-differential of a convex function that was used in order to indicate that R does not have to be smooth. Of course, the choice (3.16) restricts our attention to a specific class of material models, referred to as the *generalized standard materials*, *generalized standard models* or *generalized standard solids*, cf. Definition 3.1 below; however this class is wide enough to comprise a large number of models in plasticity (Maugin, 1992) and, in particular, all material models considered in this thesis.

Definition 3.1. [13] "A model of material behavior is a *generalized standard model* if it is defined by two potentials, the energy potential ψ and the dissipation potential R. The energy is a function of state variables and the dissipation potential is a convex function of the flux and may eventually depend on the present state." (from (Nguyen, 2000))
Furthermore, in a *generalized standard model* the dissipation potential has to be non-negative and zero for zero flux; the relation between generalized fluxes and forces is given through (3.16).

Remark 3.2 (Nomenclature). Let us note, that equation (3.16) is then sometimes (e.g. (Kružík et al., 2005; Mielke and Roubíček, 2003)), in analogy with plasticity, referred to as the *flow-rule*; we shall use this term in this thesis as well.

Further we remark that, in this work, we follow the terminology of the original paper of Halphen and Nguyen (1975) and call R a dissipation *potential* motivated by the fact that its derivative corresponds to the generalized force. On the other hand, since the change of the dissipation potential between two states is not path-independent, some authors (e.g. (Petryk, 2003)) prefer to use the name *dissipation function*.

It is easy to check that a generalized standard model, as introduced in Definition 3.1, is *thermodynamically consistent*, i.e. satisfies the second law of thermodynamics. Indeed,

$$A\cdot\dot{\alpha} = \partial_{\dot{\alpha}} R(\alpha,\dot{\alpha})\cdot\dot{\alpha} \geq R(\alpha,\dot{\alpha}) - \underbrace{R(\alpha,0)}_{0} \geq 0,$$

where the first inequality is due to *convexity*.

Remark 3.3 (Onsager reciprocity). If R is smooth, generalized standard models satisfy automatically *Onsager reciprocal relations*. (Callen, 1985)

Remark 3.4 (Relation to maximum dissipation principles). Note that the flow-rule (3.16) can be understood (when considering also the convexity) as a *minimization principle* for the dissipation potential; this minimization principle could also be stated as a postulate replacing (3.16).

Another well known postulate for formulation of constitutive function is the so-called *maximum dissipation principle* (or equivalently *maximum entropy production principle*) due to Hill (1948), recently advocated by e.g. Rajagopal and Srinivasa (2004). It has been shown by Hackl and Fischer (2008) that these two principles coincide only for some dissipation potentials, for example for those potentials that are homogeneous of degree l in the fluxes, i.e. $R(\alpha, l\dot{\alpha}) = |l|R(\alpha,\dot{\alpha})$ for any $l \in \mathbb{N}$.[14]

Remark 3.5 (Internal variables). Let us also remark, that within the framework of generalized standard solids the set of state variables $(\theta, \mathbb{Y}, \chi)$ is divided into so-called *observable variables* $(\theta, \mathbb{Y})$ and *internal variables* χ. (Maugin, 1992).[15] The motivation

[13] This definition follows (Nguyen, 2000) and is based on the original paper due to Halphen and Nguyen (1975).

[14] In (Hackl and Fischer, 2008) it was, however, also noted that if R is a sum of two functions, one of order l_1, the other of order l_2, the two principles do not need to coincide anymore; we shall use such concept in Chapter 5.

[15] Sometimes, only a part of the vector χ would be called internal.

for calling χ "internal" stems from their interpretation as variables accounting for some processes on microscale that manifest themselves on macroscale mainly through dissipation (Maugin, 1992). Consistently, in pure elastic processes the Helmholtz free energy was not allowed to depend on χ.

All in all, the procedure of formulating models within the framework of generalized standard solids is summarized by the following scheme: (Nguyen, 2000)

1. Identification of observable variables, finding the expression of the free energy.
2. Identification of dissipative processes, finding appropriate internal variables (and hence also generalized fluxes).
3. Finding a relation between generalized fluxes and forces, i.e. prescribing the dissipation potential.

After performing these steps, the evolution of the specimen is governed by the following laws *when neglecting inertia and when assuming that* $\psi = \psi(\theta, \nabla y, \chi)$

$$\operatorname{div}\big(\partial_{\nabla \dot{y}} R(\theta, \nabla y, \nabla \dot{y}, \chi, \dot{\chi}) + \psi'_{\nabla y}(\theta, \nabla y, \chi)\big) \ni 0, \tag{3.17}$$

$$\partial_{\dot{\chi}} R(\theta, \nabla y, \nabla \dot{y}, \chi, \dot{\chi}) + \psi'_{\chi}(\theta, \nabla y, \chi) \ni 0, \tag{3.18}$$

$$\theta \dot{s} + \operatorname{div}(q) = \mathcal{D} = \partial_{\nabla \dot{y}} R(\theta, \nabla y, \nabla \dot{y}, \chi, \dot{\chi}) : \nabla \dot{y} + \partial_{\dot{\chi}} R(\theta, \nabla y, \nabla \dot{y}, \chi, \dot{\chi}) \cdot \dot{\chi}, \tag{3.19}$$

where the first equation corresponds to the balance of momentum, the second to (3.16) and the third to the fact that the entropy production multiplied by temperature is, in a control volume, equal to the rate of dissipated energy, i.e. the *entropy balance*.

Examples of dissipation potentials

Let us now give two prominent examples of dissipation potentials, namely the dissipation potential for the *Kelvin-Voigt material* and for *von-Mises type elasto-plasticity*. In both cases we assume *isothermal* evolution; this corresponds to the idea that the specimen in question is kept in a basin of constant temperature and is so small that any temperature change due dissipation can be evened out instantly. Also, let us assume only the *small-eformation setting*. Finally, as already above, we assume that the evolution is *quasi-static*; so, terms corresponding to inertia can be neglected.

It is well known (see e.g. (Nguyen, 2000)) that the constitutive equation of a Kelvin-Voigt material reads (in its simplest d-dimensional form) as

$$\sigma = \mathbb{D}\dot{\varepsilon} + \mathbb{C}\varepsilon, \tag{3.20}$$

with $\varepsilon(u) = \frac{1}{2}\big(\nabla u + (\nabla u)^{\mathrm{T}}\big)$ the *small strain tensor*, $u(x) : \Omega \to \mathbb{R}^d$ the *displacement* defined as $u(x) = y(x) - x$ [16]. Furthermore, the fourth-order tensors $\mathbb{C}$ and $\mathbb{D}$ are the tensor of *elastic constants* and the tensor of *viscous moduli*, respectively. For both tensors it is natural to assume the symmetries $\mathbb{C}_{ijkl} = \mathbb{C}_{jikl} = \mathbb{C}_{ijlk} = \mathbb{C}_{klij}$ and $\mathbb{D}_{ijkl} = \mathbb{D}_{jikl} = \mathbb{D}_{ijlk} = \mathbb{D}_{klij}$.

The quasi-static evolution of the specimen is then governed by the balance of momentum [17]

$$-\operatorname{div}\sigma = f, \quad \forall x \in \Omega \tag{3.21}$$

with appropriate initial and boundary conditions.

[16] Recall that $x \in \Omega$ with Ω the reference configuration and $y(x)$ is the deformation.

[17] This corresponds to (3.2) with $\ddot{y}$ neglected and $\mathcal{P}$ identified as σ in the small strain setting.

To see that this constitutive model falls into the framework of generalized standard solids, we do not consider any internal variables χ and define the stored energy as

$$\psi(\varepsilon) = \frac{1}{2}\varepsilon^{\mathrm{T}}\mathbb{C}\varepsilon,$$

and the dissipation potential as

$$R(\dot{\varepsilon}) = \frac{1}{2}\dot{\varepsilon}^{\mathrm{T}}\mathbb{D}\dot{\varepsilon}.$$

Then (3.21) is recovered by inserting the respective potentials to (3.17) and replacing ∇y by $\varepsilon(u)$, as usual in the small deformations setting. Hence the Kelvin-Voigt material can be described by two potentials as required in Definition 3.1; the dissipation potential satisfies all requirements of the definition if $\mathbb{D}$ is *positive (semi)definite*.

For the example of *von-Mises* elasto-plasticity, we restrict ourselves, again, to the *small strain setting*. Then, the small strain tensor ε is usually decomposed into its elastic $\varepsilon_{\mathrm{el}}$ and plastic $\varepsilon_{\mathrm{pl}}$ part, i.e.

$$\varepsilon = \varepsilon_{\mathrm{el}} + \varepsilon_{\mathrm{pl}}. \tag{3.22}$$

The *plastic part of the strain tensor* is then understood to play the role of an *internal variable*. Perfect von-Mises elasto-plasticity can be then introduced by the following set of axioms (Maugin, 1992, Pages 18,54,55)

1. *There exists a strain-energy potential*[18] $\phi = \phi(\varepsilon_{\mathrm{el}})$ *such that*:

$$\sigma = \frac{\mathrm{d}\phi}{\mathrm{d}\varepsilon_{\mathrm{el}}},$$

   for the stresses σ.

2. *The stresses are constrained to a ball*[19], i.e.

$$|\sigma| \in \mathcal{C}_{\mathrm{vM}} = \{\tilde{\sigma}, |\tilde{\sigma}| \leq c_{\mathrm{vM}}\}.$$

3. *The plastic stress changes (flows) in the direction of stress only if the boundary of the elasticity domain is reached*, i.e.

$$\dot{\varepsilon}_{\mathrm{pl}} = 0 \text{ if } |\sigma| < c_{\mathrm{vM}} \qquad \text{and} \qquad \dot{\varepsilon}_{\mathrm{pl}} = \lambda\frac{\sigma}{c_{\mathrm{vM}}} \text{ if } |\sigma| = c_{\mathrm{vM}}.$$

Now realize that the conditions in point 3 can be written compactly as

$$\dot{\varepsilon}_{\mathrm{pl}} \in N_{\mathcal{C}_{\mathrm{vM}}}(\sigma) = \partial\delta_{\mathcal{C}_{\mathrm{vM}}}(\sigma), \tag{3.23}$$

with $N_{\mathcal{C}_{\mathrm{vm}}}$ and $\delta_{\mathcal{C}_{\mathrm{vM}}}$ the *normal cone* and the *indicator function* to the convex set $\mathcal{C}_{\mathrm{vm}}$, respectively. Rewriting (3.23) by exploiting the Legendre-Fenchel conjugates[20] (Rockafellar, 1970) leads to

$$\begin{aligned} -\sigma + \delta^*_{\mathcal{C}_{\mathrm{vM}}}(\dot{\varepsilon}_{\mathrm{pl}}) \ni 0 \qquad &\Leftrightarrow \qquad -\frac{\mathrm{d}\phi(\varepsilon - \varepsilon_{\mathrm{pl}})}{\mathrm{d}\varepsilon_{\mathrm{el}}} + \delta^*_{\mathcal{C}_{\mathrm{vM}}}(\dot{\varepsilon}_{\mathrm{pl}}) \ni 0 \\ &\Leftrightarrow \qquad -\frac{\mathrm{d}\phi(\varepsilon - \varepsilon_{\mathrm{pl}})}{\mathrm{d}\varepsilon_{\mathrm{pl}}} + \delta^*_{\mathcal{C}_{\mathrm{vM}}}(\dot{\varepsilon}_{\mathrm{pl}}) \ni 0. \end{aligned}$$

Note that, when identifying $\delta^*_{\mathcal{C}_{\mathrm{vM}}}(\dot{\varepsilon}_{\mathrm{pl}})$ as the dissipation potential this corresponds to (3.18); so, again, we work in the framework of generalized standard materials.

[18] This potential corresponds to the Helmholtz free energy in our setting.

[19] This ball is refered to as the elasticity domain.

[20] The Legendre-Fenchel conjugate is, for a function $f : \mathbb{R}^{M+1} \to \mathbb{R}$, defined as

$$f^*(x^*) = \sup_{x \in \mathbb{R}^{M+1}} \{(x^*, x) - f(x)\}.$$

Chapter 4

Review of existing mesoscopic models for shape-memory alloys

Recall from Chapter 1 that modeling of shape-memory alloys is a multiscale problem, modeling approaches range from the nanoscale to the polycrystalline macroscale. Within this thesis, *mesoscopic* models that are suitable for large single-crystalline specimen are our primary concern. For these models, the *microstructure* (cf. Chapter 1) is described by introducing (gradient) Young measures; physically this corresponds to the idea that "the microstructure is so fine that it can be reduced to one material point".

So far, only static models based on the pioneering works of Ball and James (1987, 1992) (see e.g. (Ball et al., 2011; Dolzmann, 2003; Müller, 1999)) and quasi-static evolutionary but *isothermal* (Bartel and Hackl, 2008, 2009; Kružík et al., 2005; Kružík and Roubíček, 2004; Mielke and Roubíček, 2003) mesoscopic models for SMAs have been proposed; we review these models within this chapter.

Besides mesoscopic models, we consider also *microscopic ones* suitable, again, for modeling single crystalline shape-memory alloys, however taking the interfacial energy of phase/variant boundaries into account and hence resolving the finite width of the microstructure. We shall show that in the static case, and later in Chapter 5 also for thermally coupled case, solutions of microscopic models approach solutions to mesoscopic models *when the interfacial energy becomes negligible.*

4.1 Static case

Recall, from Chapter 1, that $\Omega \in \mathbb{R}^d$, a regular[1] domain, is the reference configuration of the specimen which we identify with the stress-free austenitic state. Recall further that any smooth injective function $y(t) : \Omega \to \mathbb{R}^d$ such that $\det \nabla y(x,t) > 0$ is called a *deformation* of the body.

In the sequel, however, we shall relax the smoothness requirement by assuming that the deformation is an element of $W^{2,2}(\Omega;\mathbb{R}^d)$ in the case of microscopic models, in the mesoscopic case only the "average deformation" is expected to be an element of $W^{1,p}(\Omega;\mathbb{R}^d)$ with $p \in [2,\infty)$. Furthermore, we *omit the constraint on the positivity of the determinant of the deformation gradient* as relaxation theory cannot cope with this constraint up to now (cf. Chapter 2 and especially Section 2.3.2 for details).

Classically in continuum mechanics, the stable states of a specimen are assumed to be minimizers of the appropriate thermodynamic potential (see e.g. (Šilhavý, 1997)) - in the case when surface/volume forces are applied minimizers of the *Gibbs free energy* are sought, if not the appropriate potential is the *Helmholtz free energy*. Throughout

[1] We shall always assume at least Lipschitz regularity.

this thesis, we shall consider the case when surface/volume forces are taken into account and the specimen is fixed on some part of the boundary of the reference configuration $\Gamma_{\mathrm{D}} \subset \partial\Omega$ of non-zero $(d-1)$-dimensional measure. Hence, we shall work with the *Gibbs free energy*.

In order to capture the main responses of SMAs, a *constitutive choice* for the Gibbs free energy is made. For models devised for the microscopic/mesoscopic scale, usually, the complicated behavior of a SMA specimen is modeled by employing (at least implicitly) the following simplifying assumptions:

- The variants of martensite as well as the austenitic phase of the material can be distinguished by the values of ∇y (deformation gradient), i.e. the material is in variant i of martensite if $\nabla y = QU_i$ (or at least $\nabla y \approx QU_i$) and the material is in austenite if $\nabla y = Q$ (or at least $\nabla y \approx Q$) with $U_1 \dots U_M$ denoting the distortion matrices of the M variants of martensite and $Q \in \mathrm{SO}(d)$.

- When the material is (purely) in some variant of martensite or the austenitic phase, the material is *stable* (i.e. the energy is minimized).

- Phase transition can be thermally driven - i.e. above the transformation temperature, θ_{tr}, austenite is stable, below it only martensite; at θ_{tr} the phases are energetically equal.

In accordance with these assumptions the *Gibbs free energy* G is chosen to be of the following form

$$G(y,\theta) = \int_\Omega \psi(\nabla y, \theta) - f\cdot y \,\mathrm{d}x - \int_{\Gamma_{\mathrm{N}}} g\cdot y \,\mathrm{d}S, \tag{4.1}$$

where $\Gamma_{\mathrm{N}} = \partial\Omega \setminus \Gamma_{\mathrm{D}}$ (up to a null-set), f and g are the (prescribed) volume and surface force, respectively. Finally, ψ is the Helmholtz free energy which is of a multiwell character, i.e. it satisfies

$$\forall\ \theta \geq \theta_{\mathrm{tr}} \begin{cases} \psi(Q\mathbb{I},\theta) = 0 & \forall Q\ \in \mathrm{SO(d)}, \\ \psi(F,\theta) > 0 & \forall F\ \neq Q\mathbb{I},\ \forall Q\ \in \mathrm{SO(d)}, \end{cases} \tag{4.2}$$

$$\forall\ \theta \leq \theta_{\mathrm{tr}} \begin{cases} \psi(QU_i,\theta) + \delta(\theta) = 0 & \forall i = 1\dots M,\quad \forall Q\ \in \mathrm{SO(d)}, \\ \psi(F,\theta) > 0 & \forall F\ \neq QU_i\ \ \forall i = 1\dots M,\quad \forall Q\ \in \mathrm{SO(d)}, \end{cases} \tag{4.3}$$

where $\mathbb{I}$ denotes the distortion matrix of the austenite, i.e. the identity matrix and δ is an offset. The idea to use this kind of multiwell Helmholtz free energy can be found e.g. in the works (Ball and James, 1987, 1992; Dolzmann, 2003; Müller, 1999)

Since we are considering the *static case*, the temperature θ is understood to be *prescribed* throughout the specimen.

The precise form of ψ is not crucial for the discussion here, but in order to meet the frame-indifference principle ψ ahs to satify that

$$\psi(F,\theta) = \psi(QF,\theta) \qquad \text{for all } F \in \mathbb{R}^{d\times d}, \text{ all } \theta > 0 \text{ and all } Q \in \mathrm{SO}(d). \tag{4.4}$$

Consistently with this principle, some authors use e.g. a minimizing procedure to obtain a possible form of the free energy (e.g. (Kružík et al., 2005; Roubíček et al., 2007)):

$$\psi(F,\theta) = \min_{m=1\dots M+1} \psi_m, \tag{4.5}$$

with ψ_m the free energies of the austenite and the respective variants of martensite chosen, for example, in accordance with the St. Venant-Kirchhoff ansatz as

$$\psi_m(F,\theta) = \frac{1}{2}\sum_{ijkl} \epsilon^m_{ij} C^m_{ijkl} \epsilon^m_{kl} + c^m_V \theta_{\mathrm{tr}} \ln\left(\frac{\theta}{\theta_{\mathrm{tr}}}\right),$$
$$\epsilon^m = \frac{U_m^{-T} F^T F U_m^{-1} - \mathbb{I}}{2}. \tag{4.6}$$

Here C^m_{ijkl} are the elastic constants of austenite or of the respective variants of martensite.

Another approach found in literature (cf. e.g. (Bartel and Hackl, 2008, 2009) in the small strain setting) defines the Helmholtz free energy through averaging, i.e.:

$$\psi(F,\theta) = \sum_{i=1}^{M+1} \lambda_i \psi_i, \tag{4.7}$$

where $\lambda \in \mathbb{R}^{M+1}$ is the vector of volume fractions[2] and ψ_i are again the stored energies of austenite and of the variants of martensite.

Also, one could exploit the method presented in (Zimmer, 2004).

These mentioned forms of the stored energy have, for our purposes, rather an illustrative character, since the main responses of SMAs will be *qualitatively* captured by any stored energy of the form (4.2). For the sake of mathematical correctness, however, we shall demand the stored energy to be of p-growth, i.e. there exist constants c_1, c_2 such that

$$c_1(|F|^p - 1) \leq \psi(F,\theta) \leq c_2(|F|^p + 1), \tag{4.8}$$

for all $F \in \mathbb{R}^{d\times d}$, $\theta \in \mathbb{R}_+$ and some $p \in [1, \frac{2d}{d-2})$ if $d > 2$, otherwise $p \in [1,\infty)$ arbitrary.[3]

Microscopic models

Note that, the form of the Gibbs free energy proposed in (4.1) with a stored energy from (4.2) does not contain any energy contributions from the surface energy stemming from phase/variant interfaces. However such an energy contribution is essential in microscopic modeling; therefore we have to add the appropriate energy term.

Though fine approaches to determine the *interfacial energy* from elastic compatibility arguments can be found in literature (see e.g. (Maciejewski et al., 2005)), for the purposes of this thesis we adopt, as in e.g. (Bhattacharya, 2003; Müller, 1999), a very simple way to account for this energy contribution; namely, we add the second gradient to the Gibbs free energy and define (for some $\varepsilon > 0$ small)

$$\mathcal{G}^{\mathrm{S}}_\varepsilon(y,\theta) = \int_\Omega \psi(\nabla y,\theta) + \frac{\varepsilon}{2}|\nabla^2 y|^2 - f\cdot y \,\mathrm{d}x - \int_{\Gamma_{\mathrm{N}}} g\cdot y \,\mathrm{d}S. \tag{4.9}$$

An intuitive way to understand the choice of $\frac{\varepsilon}{2}|\nabla^2 y|^2$ for the interfacial energy arises from the assumption that the interfacial energy contribution manifests itself *mainly* by preventing extremely fast oscillations of the deformation gradient like in Example 2.20; so, its contribution causes the finite width of the microstructure. Indeed, due to its compactifying effect, the second gradient prevents the extremely fast oscillations.

[2] The i-th component of the vector of volume fractions describes "how much of the i-th variant of martensite/austenite is contained in the material point". Naturally, it holds that $\lambda_i \geq 0$, $i = 1 \ldots M+1$, and $\sum_{i=1}^{M+1} \lambda_i = 1$.

[3] The upper bound of p is caused by the assumed form of the interfacial energy in (4.9); by assuming a different form this bound could be arbitrarily large, but finite.

In the microscopic case, we are now in the position to rigorously formulate the minimization problem determining stable states

$$\left.\begin{array}{ll} \text{minimize} & \mathcal{G}^{\mathrm{S}}_{\varepsilon}(y,\theta) \\ \text{subject to} & y \in W^{2,2}(\Omega;\mathbb{R}^d) \quad y(x) = x \quad \text{for a.a. } x \in \Gamma_{\mathrm{D}}, \\ & \text{with } \theta \text{ prescribed,} \end{array}\right\} \tag{4.10}$$

with f and g given having the following integrability[4]

$$\left.\begin{array}{l} f \in L^{p^{*'}}(\Omega;\mathbb{R}^d) \\ g \in L^{p^{\sharp'}}(\Gamma_{\mathrm{D}},\mathbb{R}^d), \end{array}\right\} \tag{4.11}$$

where p corresponds to (4.8) and where p^*, $p^\sharp$ were specified in the Nomenclature.

Note that proving existence of solutions to (4.10) is possible, e.g. by the *direct method* (cf. (Dacorogna, 1989) or the beginning of Subsection 2.2) owing to, the already mentioned, compactifying effect of $\frac{\varepsilon}{2}|\nabla^2 y|^2$.

Mesoscopic models

For large specimen, the surface energy becomes negligible and can be omitted. To see this we provide a scaling argument following (De Simone, 1993) For simplicity, when confining ourselves only to the Helmholtz free energy and the interfacial energy[5], both integrated over the set $r\Omega$ with $|\Omega| = 1$ and $r > 0$, we have the overall free energy:

$$\begin{aligned} \int_{r\Omega} \psi(\nabla y(x),\theta(x)) + \frac{\varepsilon}{2}|\nabla^2 y(x)|^2 \,\mathrm{d}x &= \int_{r\Omega} \psi(\nabla_x y(r\tilde{x}),\theta(r\tilde{x})) + \frac{\varepsilon}{2}|\nabla_x^2 y(r\tilde{x})|^2 \,\mathrm{d}x \\ &= r^d \int_{\Omega} \psi(\nabla_x y(r\tilde{x}),\theta(r\tilde{x})) + \frac{\varepsilon}{2}|\nabla_x^2 y(r\tilde{x})|^2 \,\mathrm{d}\tilde{x} \end{aligned}$$

with $\tilde{x} \in \Omega$. Introducing the scaled deformation $\tilde{y}(\tilde{x}) = \frac{1}{r} y(r\tilde{x})$[6] and the scaled temperature $\tilde{\theta}(\tilde{x}) = \theta(r\tilde{x})$ gives finally that the energy of the large body is rescaled to a body of unit volume[7] as

$$\int_{\Omega} \psi(\nabla_{\tilde{x}} \tilde{y}(\tilde{x}),\tilde{\theta}(\tilde{x})) + \frac{\varepsilon}{2r^2}|\nabla_{\tilde{x}}^2 \tilde{y}(\tilde{x})| \,\mathrm{d}\tilde{x},$$

which shows that indeed, with $r \to \infty$, the interfacial energy goes to zero.

Let us therefore concentrate on the case when the surface energy is omitted. In this case, due to the its multiwell character, the stored energy is not quasiconvex and hence the problem

$$\left.\begin{array}{ll} \text{minimize} & G(y,\theta) \\ \text{subject to} & y \in W^{1,p}(\Omega;\mathbb{R}^d), \quad y(x) = x \quad \text{for a.a. } x \in \Gamma_{\mathrm{D}} \\ & \text{with } \theta \text{ prescibed and } G \text{ from (4.1),} \end{array}\right\} \tag{4.12}$$

may not and often[8] *will not possess solutions.* In fact, it can be expected that the infimizing sequences of $G(y,\theta)$ may exhibit very fast spatial oscillations.

[4] This integrability could be even generalized in the microscopic case. One could, for example, assume only $f \in L^a(\Omega;\mathbb{R}^d)$, with $\frac{1}{a} = \frac{1}{2} + \frac{2}{d}$ and $\frac{1}{a} = \frac{1}{2} + \frac{2}{d}$ if $d > 2$. However, since we shall need (4.11) anyhow in the mesoscopic case, we do not consider these generalizations here.

[5] So, we do not consider the extrnal force terms here.

[6] While this scaling may seem strange at the first sight, it is chosen in such a manner that the relative distortion, which is the comparable quantity is preserved.

[7] To this end, we express the derivatives with respect to x by derivatives with respect to $\tilde{x}$. Moreover, as the energy of the specimen will scale with its volume, we need to divide the energy of the body with a volume $|r\Omega|$ by r^d to rescale it to unit volume.

[8] Whether or not solutions exist will depend on the temperature θ and the prescribed forces.

Therefore, with the tools from Chapter 2, we *relax* the problem (4.12); in particular, we utilize L^p-gradient Young measures (cf. Section 2.3) to obtain[9]

$$\left.\begin{array}{ll} \text{minimize} & \mathcal{G}^{\mathrm{S}}(y,\nu,\theta)=\int_\Omega \psi(\cdot,\theta)\bullet\nu - f\cdot y\,\mathrm{d}x-\int_{\Gamma_{\mathrm{N}}} g\cdot y\,\mathrm{d}S \\ \text{subject to} & y\in W^{1,p}(\Omega;\mathbb{R}^d),\ \nu\in\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d}) \\ & \text{such that } \nabla y=\mathrm{id}\bullet\nu \text{ a.e. on } \Omega \text{ with } \theta \text{ prescribed,} \end{array}\right\} \tag{4.13}$$

Let us remind the reader that, physically, the introduced Young measures can be interpreted as representants of microstructure so fine that it can be "reduced to a material point".

Assuming (4.8) for ψ and (4.11), the relaxed problem (4.13) possesses, exploiting Theorem 2.19 in Chapter 2, solutions. As already stressed in Example 2.20, the minimizer also contains some information about the infimizing sequence.

To end this section, let us show that gradients of solutions to (4.10) generate *some, perhaps not all,* minimizers of (4.13).

Proposition 4.1. *Let (4.8) and (4.11) hold. Let $y_\varepsilon\in W^{2,2}(\Omega;\mathbb{R}^d)$ be the solutions to (4.10). Then there exists a subsequence of ε (not relabeled) and a couple $(y,\nu)\in W^{1,p}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^d)\times\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d})$ such that $y_\varepsilon\rightharpoonup y$ in $W^{1,p}(\Omega;\mathbb{R}^d)$ and ∇y_ε generates ν. Furthermore, $\nabla y=\mathrm{id}\bullet\nu$ a.e. on Ω and (y,ν) solve (4.13).*

Proof. By testing the minimization problem (4.10) e.g. by $y(x)=x$ in can be seen that $\mathcal{G}^{\mathrm{S}}_\varepsilon(y_\varepsilon,\theta)$ is uniformly bounded in $\mathbb{R}$ and hence, by the coercivity (4.8), y_ε is uniformly bounded in $W^{1,p}(\Omega;\mathbb{R}^d)$. Thanks to the Banach selection principle and to Theorem 2.9, we select a subsequence of ε (not relabeled) and a couple $(y,\nu)\in W^{1,p}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^d)\times\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d})$ such that $y_\varepsilon\rightharpoonup y$ in $W^{1,p}(\Omega;\mathbb{R}^d)$ (thanks to the bound on $\{\nabla y_\varepsilon\}_{\varepsilon>0}$ and the Dirichlet boundary condition) and ∇y_ε generates ν.

Since id is of linear growth – and hence an element of $C_p(\Omega;\mathbb{R}^{d\times d})$[10]– $\int_\Omega \nabla y_\varepsilon(x)\chi(x)\,\mathrm{d}x \to \int_\Omega \mathrm{id}\bullet\nu(x)\chi(x)\,\mathrm{d}x$, for any $\chi\in L^\infty(\Omega)$, which readily yields $\nabla y=\mathrm{id}\bullet\nu$ a.e. on Ω.

It only remains to show that (y,ν) solve (4.13). To this end we exploit Lemma 2.11 and the non-negativity of $\frac{\varepsilon}{2}|\nabla^2 y(x)|^2$ to get

$$\begin{aligned}\mathcal{G}^{\mathrm{S}}(y,\nu,\theta)&\le\liminf_{\varepsilon\to0}\int_\Omega \psi(\nabla y_\varepsilon,\theta)-f\cdot y_\varepsilon\,\mathrm{d}x-\int_{\Gamma_{\mathrm{N}}} g\cdot y_\varepsilon\,\mathrm{d}S\\ &\le\liminf_{\varepsilon\to0}\int_\Omega \psi(\nabla y_\varepsilon,\theta)+\frac{\varepsilon}{2}|\nabla^2 y(x)|^2-f\cdot y_\varepsilon\,\mathrm{d}x-\int_{\Gamma_{\mathrm{N}}} g\cdot y_\varepsilon\,\mathrm{d}S=\mathcal{G}^{\mathrm{S}}_\varepsilon(y_\varepsilon,\theta).\end{aligned}$$

Since y_ε solves (4.10) we have that

$$\liminf_{\varepsilon\to0}\mathcal{G}^{\mathrm{S}}_\varepsilon(y_\varepsilon,\theta)\le\liminf_{\varepsilon\to0}\mathcal{G}^{\mathrm{S}}_\varepsilon(\tilde y,\theta)=\int_\Omega \psi(\tilde y,\theta)-f\cdot\tilde y\,\mathrm{d}x-\int_{\Gamma_{\mathrm{N}}} g\cdot\tilde y\,\mathrm{d}S$$

for any $\tilde y\in W^{2,2}(\Omega;\mathbb{R}^d)$. Now choose any $\bar\nu\in\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d})$ and a corresponding $\bar y\in W^{1,p}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^d)$ with $\nabla\bar y=\mathrm{id}\bullet\bar\nu$ a.e. on Ω. Then, due to Lemma 2.18, $\bar\nu$ can be generated by a sequence $y_k\in W^{1,p}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^d)$ such that $|\nabla y_k|^p$ is weakly convergent in $L^1(\Omega)$; by mollifier arguments one could even assume that $y_k\in W^{2,2}(\Omega;\mathbb{R}^d)$ without destroying the weak convergence of $|\nabla y_k|^p$ in $L^1(\Omega)$. Choosing therefore $\tilde y=y_k$ in the already proved relation

$$\mathcal{G}^{\mathrm{S}}(y,\nu,\theta)\le\int_\Omega \psi(\tilde y,\theta)-f\cdot\tilde y\,\mathrm{d}x-\int_{\Gamma_{\mathrm{N}}} g\cdot\tilde y\,\mathrm{d}S,$$

and passing to the limit $k\to\infty$ gives the claim. □

[9] This relaxation approach is due to Ball and James (1987, 1992).

[10] Recall that we assume $p\in[1,\frac{2d}{d-2})$ if $d>2$, otherwise $p\in[1,\infty)$.

Let us stress that, while this proposition justifies the mesoscopic approach since it shows that it is a good approximation for the case the interfacial energy becomes negligible, it *does not imply* that $\mathcal{G}^{\mathrm{S}}$ is the Γ-limit of $\mathcal{G}^{\mathrm{S}}_{\varepsilon}$ when $\varepsilon \to 0$.

4.2 Mesoscopic models in the isothermal quasi-static rate-independent case

Finding stable states of a SMA specimen, when exposed to given loads, offers insight into its behavior, but generalizations of the static models also to the evolutionary case on the microscopic/mesoscopic scale are desirable to be able to model loading cycles. Therefore, evolutionary mesoscopic models for SMAs have been proposed in e.g. (Bartel and Hackl, 2008, 2009; Kružík et al., 2005; Kružík and Zimmer, 2011; Mielke and Roubíček, 2003; Roubíček et al., 2007). Let us stress, however, that all these works consider the *isothermal* case or consider with *temperature as a given prescribed load*. (see e.g. (Mielke and Petrov, 2007)).

In this review, we follow the approach of (Kružík et al., 2005; Roubíček et al., 2007), since ideas from these papers will be extended in Chapter 5 for thermally coupled case; still, we point to other works on modeling of evolution on other scales whenever appropriate.

As confirmed by many experiments (see e.g. the review paper (Otsuka and Ren, 2005)), when the state of an SMA specimen evolves and, in particular, when its internal structure changes, energy is dissipated; this manifests itself by a pronounced hysteresis in stress/ temperature/strain loading cycles. Any generalization of static models should, therefore, be able to capture this hysteresis effect.

Realize that it is exactly this dissipation mechanism that makes the response of a SMA specimen *path-dependent*, i.e. the currently observed state of the specimen (which might even seem stable) *does depend on the way how this state was reached*. An interesting experimental confirmation of this fact was given in (Seiner et al., 2009; Seiner and Landa, 2009) (and analyzed in (Ball et al., 2009)) where a so-called *X-interface* in a *CuAlNi*-single crystal was observed that *does not correspond* to any stable state obtained solving (4.13). The deviation from a stable state predicted by (4.13) is small but still supports the necessity of including dissipation mechanisms into the model.

Some authors (cf. (Kružík et al., 2005) for a review) try to model this dissipation also through the stored-energy landscape. It assumed that, if the orbits $\mathrm{SO}(d)U_i$ and $\mathrm{SO}(d)U_j$ are rank-1 connected, then dissipation of a phase transition between these variants is small, or rather zero – otherwise dissipation is related with metastability.

Especially authors developing macroscopic models rely rather on the idea that the dissipation mechanism needs to be described by a separate phenomenology (recording, e.g, impurities and dislocations etc.) (cf. e.g. (Auricchio et al., 2007; Lagoudas et al., 2011; Lexcellent et al., 2000, 1994; Rajagopal and Srinivasa, 1999; Sadjadpour and Bhattacharya, 2007*a*,*b*)).

In the spirit of works (Kružík et al., 2005; Mielke and Roubíček, 2003), which we aim to extend, we shall follow the second approach, but some ideas from the first one are reflected, too.

Indeed, Kružík et al. (2005); Mielke and Roubíček (2003) work within the framework of *generalized standard materials* and hence have to carry out the steps specified in Section 3.2, i.e. identify a suitable set of state variables as well as define the appropriate energy and dissipation potential.

Since Kružík et al. (2005); Mielke and Roubíček (2003) are concerned *mesoscopic* models, and the authors understand their work as an extension of the concepts presented in Section 4.1, the "averaged" deformation $y \in W^{1,p}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^d)$ and the gradient Young

measure $\nu \in \mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^{d\times d})$ were selected as a state variables. Furthermore, an internal variable, namely the *the vector of volume fractions* λ, was introduced – the component $\lambda_i(x)$ of which represents the ratio of the i-th's variant of martensite ($i = 1 \dots M$[11]) and $\lambda_{M+1}(x)$ the ratio of austenite contained in the material point x. Therefore, one assumes $\lambda \in L^\infty(\Omega;\mathbb{R}^{M+1})$ and $\lambda_i(x) \geq 0$ and $\sum_{i=1}^{M} \lambda_i(x) = 1$ for a.a. $x \in \Omega$.[12]

Recall, that the state variable ν can be conceptually understood as "infinitely fine microstructure"; so, it is natural to impose a connection between the vector of volume fractions and ν. In (Kružík et al., 2005; Mielke and Roubíček, 2003) this connection was expressed by introducing a function $L : \mathbb{R}^{d\times d} \to \mathbb{R}^{M+1}$ and putting

$$\lambda(x) = L \bullet \nu_x \qquad \text{for a.a. } x \in \Omega. \tag{4.14}$$

When describing the dissipation, the authors of (Kružík et al., 2005; Mielke and Roubíček, 2003) pursued the modeling assumption that *only changes in the ratio of the respective phases and/or variants in a material points are dissipative* but not purely geometric changes that preserve the vector of volume fractions. This is clearly a simplification, since if a geometric change occurs a rearrangement of atoms in the crystal lattice is needed, similarly as when their ratio changes. Hackl and Kochmann (Hackl and Kochmann, 2008) address this issue for laminates in crystal plasticity; we, however, accept this simplification following (Kružík et al., 2005; Mielke and Roubíček, 2003) having also in mind that geometric changes are usually not observed in experiments (see e.g (Bartel and Hackl, 2009)).

The dissipation mechanism is then modeled by prescribing a dissipation potential density $r : \mathbb{R}^{M+1} \mapsto \mathbb{R}$ which depends on $\dot\lambda$ *only*, i.e. $r = r(\dot\lambda)$. Again, this is a simplification since the dissipation may well depend on the current state of the material. However, the state dependence of the dissipation potential is not explored well enough up to now and was, to the authors' knowledge, taken into account only in macroscopic models e.g. (Sedlák et al., 2012).

In order to capture that the martensitic transformation and martensite reorientation are *activated* processes, r has to be non-smooth at 0. Moreover, r was chosen to be homogeneous of degree 1 in (Kružík et al., 2005; Mielke and Roubíček, 2003) as their modeling approach followed the often used rate-independent approximation (also used in e.g. (Arndt et al., 2006; Aubry et al., 2003; Auricchio and Petrini, 2002; Bartel and Hackl, 2008, 2009; Lexcellent et al., 1994; Petryk and Stupkiewicz, 2010; Petryk et al., 2010; Sadjadpour and Bhattacharya, 2007*b*) and many others).

As long as one-homogeneity is guaranteed, from the mathematical point of view, no further assumptions have to be put on the dissipation potential; prescribing a specific form is not necessary for performing the existence analysis. Yet, in the precise form of the dissipation potential the idea that dissipation should be small if a transition proceeds between two variants of martensite, the distortion matrices of which are rank-1 connected (cf. (Kružík et al., 2005)), can be reflected – indeed, for most of the known SMA-materials distortion matrices corresponding to any two variants of martensite are rank-1 connected (see e.g. (Bhattacharya, 2003)). Then, when choosing $R(\cdot)$ for example as [13]

$$r(\dot\lambda) = \sum_{i=1}^{M+1} \gamma_i |\dot\lambda_i|, \tag{4.15}$$

one could set γ_i for $i = 1 \dots M$ small compared to γ_{i+1}. However, note that because of the experimental evidence of martensite stabilization mentioned in Chapter 1 (Liu and

[11] Recall that M is the number of martensitic variants.

[12] In mathematics, however, we shall enforce these constrains through the function L defined in (4.14).

[13] Precisely this form has been chosen in (Kružík et al., 2005) to perform calculations.

Favier, 2000; Picornell et al., 2006) the coefficients γ_i should not be set to 0 even for $i = 1 \dots M$.

The dissipation potential is then, by means of its density, defined as

$$R^{\mathrm{RI}}(\dot{\lambda}) = \int_\Omega r(\dot{\lambda}) \,\mathrm{d}x. \tag{4.16}$$

In accordance with the static case, the following form of the Gibbs free energy has been chosen (here already relaxed by means of gradient Young measures)

$$\mathcal{G}^{\mathrm{RI}}(t, y, \nu, \theta) = \int_\Omega \psi(\cdot, \theta) \bullet \nu - f(t) \cdot y \,\mathrm{d}x - \int_{\Gamma_{\mathrm{N}}} g(t) \cdot y \,\mathrm{d}S + \delta \left\| \lambda \right\|^r_{\alpha,r}, \tag{4.17}$$

where ψ could be chosen as in (4.2) [14] and $\|\lambda\|^r_{\alpha,r}$ is the norm in the Sobolev-Slobodeckii space $W^{\alpha,r}(\Omega; \mathbb{R}^{M+1})$ and $\delta > 0$. Note that this form corresponds to the one presented in (4.13) except for the norm of the space with fractional derivatives $W^{\alpha,r}(\Omega; \mathbb{R}^{M+1})$. This norm can be linked to some capillarity-like effects (Kružík et al., 2005), however the authors include it mostly for reasons of mathematical consistency - without it, they would not have enough regularity at disposal to prove existence of solutions.

Note also, that since (4.17) refers to an energy for an evolutionary problem the Gibbs free energy also depends directly on the *time* $t \in [0, T]$.

Following (3.17)-(3.18) the evolution of the specimen is then governed by the following inclusions

$$\partial_\nu \big(\mathcal{G}^{\mathrm{RI}}(t, y, \nu, \lambda) + \delta_{\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega; \mathbb{R}^{d\times d})}(\nu) \big) \ni 0, \tag{4.18}$$

$$\partial R^{\mathrm{RI}}(\dot{\lambda}) + [\mathcal{G}^{\mathrm{RI}}]'_\lambda(t, y, \nu, \lambda) \ni 0, \tag{4.19}$$

with y uniquely through the relations $\nabla y = \mathrm{id} \bullet \nu$, $y = x$ on Γ_{D}. We furthermore prescribe the initial conditions

$$y(0, \cdot) = y_0, \qquad \nu(0, \cdot) = \nu_0, \qquad \lambda(0, \cdot) = \lambda_0 \qquad \text{on} \quad \Omega, \tag{4.20}$$

that are again compatible in the sense that $\nabla y_0 = \mathrm{id} \bullet \nu_0$.

Now, since the $\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega; \mathbb{R}^{d\times d})$ is *not a convex set*, the subdifferentials in (4.18)-(4.19) are understood rather formally; hence it is necessary to formulate (4.18)-(4.19) appropriately *weakly*. An advantageous weak formulation to this kind of *doubly nonlinear problems* was proposed by Mielke and Theil in (Mielke and Theil, 2004) and is referred to as the *energetic formulation*, see also the related works (Mainik and Mielke, 2005; Mielke, 2005; Mielke and Theil, 2004; Mielke and Levitas, 2002). This approach was taken also by the authors of (Kružík et al., 2005; Mielke and Roubíček, 2003) and the following concept of solutions was defined:

Definition 4.2. [15] Assume that $L(\cdot)_i \geq 0$ for $i = 1 \dots M+1, \sum_{i=1}^{M+1} L(\cdot)_i = 1$[16]. Then, the triple $(y, \nu, \lambda) : [0, T] \to \mathcal{Q}^c$ with

$$\mathcal{Q} = \Big\{ (\tilde{y}, \tilde{\nu}, \tilde{\lambda}) \in W^{1,p}(\Omega, \mathbb{R}^d) \times \mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega; \mathbb{R}^{d\times d}) \times W^{\alpha,r}(\Omega, \mathbb{R}^{M+1}) \text{ such that } \nabla y = \mathrm{id} \bullet \nu \Big\}$$

$$\mathcal{Q}^c = \Big\{ (\tilde{y}, \tilde{\nu}, \tilde{\lambda}) \text{ such that } \tilde{\lambda} = L \bullet \tilde{\nu} \text{ for a.a. } x \in \Omega \Big\}$$

[14] In fact, the authors of (Kružík et al., 2005) chose the form as in (4.5)-(4.6) for their calculations, however their existence analysis is valid under general assumptions of continuity and p-growth of ψ, cf. Proposition 4.3 below.

[15] Following (Kružík et al., 2005; Mielke and Roubíček, 2003) and the concept of *energetic solutions* as presented in e.g. (Mielke, 2005; Mielke and Theil, 2004; Mielke and Levitas, 2002).

[16] Note that we shall drop the requirement for the vector of volume fraction λ that $\lambda_i \geq 0$ for $i = 1 \dots M+1, \sum_{i=1}^{M+1} \lambda_i = 1$ and rather imposed it through the function L; this procedure shall be again exploited in Chapter 5.

will be called an energetic solution to the (4.18)-(4.19) with initial conditions (4.20), if it satisfies

1. *the stability condition*:

$$\mathcal{G}^{\mathrm{RI}}(t,y,\nu,\lambda) \le \mathcal{G}^{\mathrm{RI}}(t,\tilde{y},\tilde{\nu},\tilde{\lambda}) + R^{\mathrm{RI}}(\lambda-\tilde{\lambda}), \tag{4.21}$$

   for any $(\tilde{y},\tilde{\nu},\tilde{\lambda}) \in \mathcal{Q}^c$ and all $t \in [0,T]$,

2. *the energetic equality*: whenever $q(t) \in \mathcal{Q}^c$ then $\partial_t \mathcal{G}^{\mathrm{RI}}(t,y,\nu,\lambda)$ exists, is continuous and moreover

$$\begin{aligned}\mathcal{G}^{\mathrm{RI}}(T,y(T),\nu(T),\lambda(T)) + \mathrm{Var}_{R^{\mathrm{RI}}}(\lambda;\Omega\times[0,T])\\ = \mathcal{G}^{\mathrm{RI}}(0,y_0,\nu_0,\lambda_0) + \int_0^T [\mathcal{G}^{\mathrm{RI}}]'_t(t,y(s))\mathrm{d}s,\end{aligned} \tag{4.22}$$

   when realizing that actually $[\mathcal{G}^{\mathrm{RI}}]'_t(t,y(s),\nu(s),\lambda(s)) = [\mathcal{G}^{\mathrm{RI}}]'_t(t,y(s))$ and where Var_f denotes the variation in time of a functions φ with respect to f defined as

$$\begin{aligned}\mathrm{Var}_f(\phi;B\times[t_1,t_2]) = \sup\Big\{ \sum_i \int_B f(\phi(t^i,x)-\phi(t^{i-1},x))\,\mathrm{d}x;\\ \text{for all partitions } t_1 \le t^1 \le t^2 \ldots \le t^n \le t_2\Big\}.\end{aligned} \tag{4.23}$$

and the initial condition (4.20).

In (Kružík et al., 2005; Mielke and Roubíček, 2003) the existence of *energetic solutions* (4.18)-(4.19) with initial conditions (4.20) under appropriate integrability conditions on data and continuity/growth conditions on the potential could be proved. We summarize, for the readers convenience, the statements of (Kružík et al., 2005; Mielke and Roubíček, 2003) in Proposition 4.3 and provide a short sketch of proof.

Proposition 4.3. [17] *Assume that $\alpha > 0$, $r > 1$ $\psi \in C(\mathbb{R}^{d\times d}\times\mathbb{R}_+)$ satisfies (2.3) and*

$$\text{there exist constants } e_1, e_2 \text{ s.t.} \quad e_1|\cdot| \le r(\cdot) \le e_2|\cdot| \tag{4.24}$$

$$f \in W^{1,1}([0,T],L^{p^*{}'}(\Omega,\mathbb{R}^d)) \tag{4.25}$$

$$g \in W^{1,1}([0,T],L^{p^\sharp{}'}(\Gamma_{\mathrm{N}},\mathbb{R}^d)) \tag{4.26}$$

$$(y_0,\nu_0,\lambda_0) \in \mathcal{Q}^c. \tag{4.27}$$

Then there exists an energetic weak solution to (4.18)-(4.19) with initial conditions (4.20).

Short sketch of proof. The proof in (Kružík et al., 2005) follows the general framework proposed in the works of Francfort and Mielke (2006) and Mielke and Theil (2004) and is performed within five steps. Here we give just a short sketch to highlight the main ideas and refer the reader to the original papers (Kružík et al., 2005; Mielke and Roubíček, 2003) for further details.

Step 1: Formulation of a time-incremental problem
Let us discretize the time with a time-step τ and introduce the so-called *time-incremental minimization problem* in every time-step; this problem is the discrete counterpart to (4.21) and (4.22).

[17] Taken from (Kružík et al., 2005).

Hence, we call the triple $(y_\tau^k, \nu_\tau^k, \lambda_\tau^k) \in \mathcal{Q}$ the *discrete weak solution* of (4.18)-(4.19) at time-level k, $k = 1 \dots T/\tau$, if it satisfies:

$$\left.\begin{array}{ll} \text{Minimize} & \mathcal{G}^{\mathrm{RI}}(t_k, y, \nu, \lambda) + \dfrac{1}{\tau}\|\lambda - L \bullet \nu\|_{H^{-1}(\Omega;\mathbb{R}^{M+1})} + R^{\mathrm{RI}}(\lambda - \lambda_\tau^{k-1}) \\ \text{subject to} & (y, \nu, \lambda) \in \mathcal{Q} \text{ with } \lambda_\tau^{k-1} \text{ obtained at time-level } k-1, \end{array}\right\} \tag{4.28}$$

where we abbreviated $t_k = k\tau$.

Note that, in this discrete formulation, the constraint $\lambda = L \bullet \nu$ was dropped (hence we are using the space $\mathcal{Q}$ instead of $\mathcal{Q}^c$ for the search of minimizers) and instead the penalization $\frac{1}{\tau}\|\lambda - L \bullet \nu\|_{H^{-1}(\Omega;\mathbb{R}^{M+1})}$ was introduced. Therefore, λ and ν are, for the moment, decoupled which allows for using the direct method to prove existence of solutions to (4.28).

For further convenience, let us also denote

$$\mathcal{G}_\tau^{\mathrm{RI}}(t, y, \nu, \lambda) = \mathcal{G}^{\mathrm{RI}}(t, y, \nu, \lambda) + \frac{1}{\tau}\|\lambda - L \bullet \nu\|_{H^{-1}(\Omega;\mathbb{R}^{M+1})}.$$

Step 2: A-priori estimates

Let us define the backward *piecewise constant interpolants* y_τ, ν_τ and λ_τ as

$$\big[y_\tau, \nu_\tau, \lambda_\tau\big](t) = \big(y_\tau^k, \nu_\tau^k, \lambda_\tau^k\big) \qquad \text{for } \ (k-1)\tau < t \le k\tau, \ \ k = 1, ..., T/\tau. \tag{4.29}$$

Then these interpolants satisfy the following bounds (here and in the following we use C as a *generic constant* that does not depend on τ):

$$\sup_{t\in[0,T]} |\mathcal{G}_\tau(t, \nu_\tau(t), y_\tau(t), \lambda_\tau(t))| \le C, \tag{4.30}$$

$$\sup_{t\in[0,T]} \|y_\tau\|_{W^{1,p}(\Omega;\mathbb{R}^d)} \le C, \tag{4.31}$$

$$\sup_{t\in[0,T]} \Big\| |\cdot|^p \bullet \nu_\tau \Big\|_{L^1(\Omega;\mathbb{R}^d)} \le C, \tag{4.32}$$

$$\|\lambda_\tau\|_{BV([0,T],L^1(\Omega;\mathbb{R}^{M+1}))\cap L^\infty([0,T];W^{\alpha,r}(\Omega,\mathbb{R}^{M+1}))} \le C. \tag{4.33}$$

Moreover a discrete stability condition

$$\mathcal{G}_\tau^{\mathrm{RI}}(t_k, y_\tau(t_k), \nu_\tau(t_k), \lambda_\tau(t_k)) \le \mathcal{G}_\tau^{\mathrm{RI}}(t_k, \tilde{y}, \tilde{\nu}, \tilde{\lambda}) + R^{\mathrm{RI}}(\lambda_\tau(t_k) - \tilde{\lambda}) \quad \forall\ (\tilde{y}, \tilde{\nu}, \tilde{\lambda}) \in \mathcal{Q}, \tag{4.34}$$

and the discrete two-sided energy inequality

$$\begin{aligned} \int_0^{t_l} [\mathcal{G}^{\mathrm{RI}}]_t'(s, y_\tau(t_k))\mathrm{d}s \le \mathcal{G}_\tau^{\mathrm{RI}}(t_k, y_\tau(t_k), \nu_\tau(t_k), \lambda_\tau(t_k)) + \mathrm{Var}_{R^{\mathrm{RI}}}(\lambda_\tau; \Omega \times [0,T]) \\ -\mathcal{G}_\tau(0, y_0, \nu_0, \lambda_0) \le \int_0^{t_l} [\mathcal{G}^{\mathrm{RI}}]_t'(s, y_\tau(t_{k-1}))\mathrm{d}s, \end{aligned} \tag{4.35}$$

for any $l \in 1 \dots T/\tau$ can be proved.

The bounds (4.30) - (4.33) are obtained by testing (4.28) with the initial conditions; note also that for the initial conditions we have $\lambda_0 = L \bullet \nu_0$; so, the estimates are really uniform in τ. We refer to (Kružík et al., 2005) for details.

As to (4.34), note that the convexity and one-homogeneity of R^{RI} assure the *triangle inequality* $R^{\mathrm{RI}}(\lambda_1 + \lambda_2) \le R^{\mathrm{RI}}(\lambda_1) + R^{\mathrm{RI}}(\lambda_2)$ to be satisfied, cf. e.g. (Mielke and Rossi, 2007). Therefore, one can test (4.28) by any $(\tilde{y}, \tilde{\nu}, \tilde{\lambda}) \in \mathcal{Q}$ to get (see e.g. (Francfort and Mielke, 2006; Kružík et al., 2005; Mielke and Theil, 2004))

$$\mathcal{G}_\tau^{\mathrm{RI}}(t_k, y_\tau(t_k), \nu_\tau(t_k), \lambda_\tau(t_k)) + R^{\mathrm{RI}}(\lambda_\tau(t_k) - \lambda_\tau(t_{k-1})) \le \mathcal{G}_\tau^{\mathrm{RI}}(t_k, \tilde{y}, \tilde{\nu}, \tilde{\lambda}) + R^{\mathrm{RI}}(\tilde{\lambda} - \lambda_\tau(t_{k-1})),$$

which, by using the triangle, inequality leads to (4.34).

In order to show (4.35), test (4.28) by $(y_\tau(t_{k-1}), \nu_\tau(t_{k-1}), \lambda_\tau(t_{k-1}))$ to get

$$\mathcal{G}_\tau^{\mathrm{RI}}(t_k, y_\tau(t_k), \nu_\tau(t_k), \lambda_\tau(t_k)) + R^{\mathrm{RI}}(\lambda_\tau(t_k) - \lambda_\tau(t_{k-1})) \le \mathcal{G}_\tau^{\mathrm{RI}}(t_k, , y_\tau(t_{k-1}), \nu_\tau(t_{k-1}), \lambda_\tau(t_{k-1}))$$
$$= \mathcal{G}_\tau^{\mathrm{RI}}(t_{k-1}, , y_\tau(t_{k-1}), \nu_\tau(t_{k-1}), \lambda_\tau(t_{k-1})) + \int_{t_{k-1}}^{t_k} [\mathcal{G}^{\mathrm{RI}}]_t'(s, y_\tau(t_{k-1}))\mathrm{d}s.$$

Summing this from 1 to l gives exactly the second part in (4.35). Moreover, as we know that $(y_\tau(t_{k-1}), \nu_\tau(t_{k-1}), \lambda_\tau(t_{k-1}))$ satisfies the discrete stability condition (4.34), we have

$$\begin{aligned}
&\mathcal{G}_\tau^{\mathrm{RI}}(t_{k-1}, y_\tau(t_{k-1}), \nu_\tau(t_{k-1}), \lambda_\tau(t_{k-1})) \\
&\quad \le \mathcal{G}_\tau^{\mathrm{RI}}(t_{k-1}, y_\tau(t_k), \nu_\tau(t_k), \lambda_\tau(t_k)) + R^{\mathrm{RI}}(\lambda_\tau(t_k) - \lambda_\tau(t_{k-1})) \\
&\quad = \mathcal{G}_\tau^{\mathrm{RI}}(t_k, y_\tau(t_k), \nu_\tau(t_k), \lambda_\tau(t_k)) - \int_{t_k}^{t_{k-1}} [\mathcal{G}^{\mathrm{RI}}]_t'(s, y_\tau(t_k),)\mathrm{d}s + R^{\mathrm{RI}}(\lambda_\tau(t_k) - \lambda_\tau(t_{k-1})),
\end{aligned}$$

which, when summing again from 1 to l, gives exactly the first part of the discrete energy inequality.

Step 3: Selecting subsequences

Due to the estimate (4.33), we may find, by an application of Helly's selection principle in its slightly generalized form (cf. (Mainik and Mielke, 2005)), a subsequence of τ's (not relabeled) and $\lambda \in BV([0,T]; L^1(\Omega; \mathbb{R}^{M+1})) \cap L^\infty([0,T]; W^{\alpha,r}(\Omega, \mathbb{R}^{M+1}))$ such that $\lambda_\tau(t) \rightharpoonup \lambda(t)$ in $W^{\alpha,r}(\Omega; \mathbb{R}^{M+1})$ for all $t \in [0,T]$.

Thanks to estimate (4.30), $\mathcal{G}_\tau^{\mathrm{RI}}(T, y_\tau(T), \nu_\tau(T), \lambda_\tau(T))$ converges to a limit, say $\mathcal{G}^{\mathrm{RI}}(T) \in \mathbb{R}$; after possibly choosing a further subsequence of τ's.

Also, as the collection of measurable function $[\mathcal{G}^{\mathrm{RI}}]_t'(t, y_\tau)$ is, due to (4.31), uniformly in τ bounded from above by yet another measurable function, we get by Fatou's lemma that[18]

$$\limsup_{\tau \to 0} \int_0^T [\mathcal{G}^{\mathrm{RI}}]_t'(s, y_\tau)\, \mathrm{d}s \le \int_0^T \limsup_{\tau \to 0} [\mathcal{G}^{\mathrm{RI}}]_t'(s, y_\tau)\, \mathrm{d}s.$$

Fix some $t \in [0,T]$. Then, we select a t-dependent subsequence of τ's denoted τ_t such that

$$\limsup_{\tau \to 0} [\mathcal{G}^{\mathrm{RI}}]_t'(t, y_\tau) = \lim_{\tau_t \to 0} [\mathcal{G}^{\mathrm{RI}}]_t'(t, y_\tau).$$

From this time-dependent subsequence, we select yet another subsequence (which we do no relabel, however) such that $\nu_{\tau_t}(t) \overset{*}{\rightharpoonup} \nu(t)$ in $\mathscr{G}_{\Gamma_{\mathrm{D}}}(\Omega; \mathbb{R}^{d\times d})$ and $y_{\tau_t}(t) \rightharpoonup y(t)$ in $W^{1,p}(\Omega; \mathbb{R}^d)$ such that $y(t) = x$ on Γ_{D} and $\nabla y(t) = \mathrm{id} \bullet \nu(t)$ a.e. on Ω.

In particular, the limit $y(t)$ satisfies

$$\limsup_{\tau \to 0} \int_0^T [\mathcal{G}^{\mathrm{RI}}]_t'(s, y_\tau)\, \mathrm{d}s \le \int_0^T [\mathcal{G}^{\mathrm{RI}}]_t'(s, y)\, \mathrm{d}s, \tag{4.36}$$

details in (Kružík et al., 2005; Mainik and Mielke, 2005); a similar procedure will be also performed in *Step 1* of the proof Theorem 5.12.

Finally, we realize that due to (4.30) $\lambda(t) = L \bullet \nu(t)$ for all $t \in [0,T]$ and so, in particular, $(y(t), \nu(t), \lambda(t)) \in \mathcal{Q}^c$.

Step 4: Passing to the limit in the discrete stability condition

Realizing that if $\lambda_\tau(t) \rightharpoonup \lambda(t)$ in $W^{\alpha,r}(\Omega; \mathbb{R}^{M+1})$ then also $\lambda_\tau(t) \to \lambda(t)$ in $L^1(\Omega; \mathbb{R}^{M+1})$, leads to the observation that $R^{\mathrm{RI}}(\lambda_\tau(t) - \tilde{\lambda}) \to R^{\mathrm{RI}}(\lambda(t) - \tilde{\lambda})$ for any $\tilde{\lambda} \in \mathbb{R}^{M+1}$. This

[18] This procedure is inspired by (Dal Maso et al., 2005) and was used in (Kružík et al., 2005), however not in (Mielke and Roubíček, 2003) where instead a so-called *non-buckling* condition was introduced.

and the weak lower semi-continuity in the Gibbs free energy allow usto keep the time $t \in [0,T]$ fixed and pass to the limit $\tau_t \to 0$ in (4.34) to obtain (4.21). Note that this procedure also gives the $\mathcal{G}^{\mathrm{RI}}(T) = \mathcal{G}^{\mathrm{RI}}(T, y(T), \nu(T), \lambda(T))$ with $\mathcal{G}^{\mathrm{RI}}(T)$ defined in Step 3.

Step 5: Passing to the limit in the lower energy inequality
Exploiting that $\mathcal{G}^{\mathrm{RI}}_\tau(T, y_\tau(T), \nu_\tau(T), \lambda_\tau(T)) \to \mathcal{G}^{\mathrm{RI}}(T, y(T), \nu(t), \lambda(T))$, the weak lower semi-continuity of the variation and the relation (4.36) allows for a limit pasage $\tau \to 0$ in the lower inequality of (4.35) yielding (cf. (Kružík et al., 2005) for details)

$$\mathcal{G}^{\mathrm{RI}}(T, y(T), \nu(T), \lambda(T)) - \mathcal{G}(0, y_0, \nu_0, \lambda_0) + \mathrm{Var}_{R^{\mathrm{RI}}}(\lambda; \Omega \times [0,T]) \le \int_0^T [\mathcal{G}^{\mathrm{RI}}]'_t(s, y(s)) \mathrm{d}s.$$

Step 5: Establishing the energy inequality
The opposite inequality in (4.22) is actually a consequence of the stability as realized in e.g. (Kružík et al., 2005). □

Chapter 5

Thermally coupled extension of mesoscopic SMA models

Most existing evolutionary mesoscopic models (e.g. (Bartel and Hackl, 2008, 2009; Kružík et al., 2005; Mielke and Roubíček, 2003; Roubíček et al., 2007)), in particular those reviewed in Section 4.2, consider the *temperature as fixed*. Clearly, this assumption rules out modeling of heating and cooling of the specimen and hence one of the most important responses of SMAs, the *shape-memory effect*, cannot be captured by these models. To overcome this issue, a rather straightforward extensions of the model reviewed in Section 4.2 with temperature as an prescribed load can be formulated based on (Mielke et al., 2009; Mielke and Petrov, 2007). Although this extension might be suitable for very small specimen, where one can assume that temperature changes can be compensated very fast and hence the temperature within the specimen is practically equal to the one prescribed on the boundary, for larger specimen this approach is again insufficient. Rather, including *thermomechanic coupling* into the model that would allow us to prescribe the temperature on the boundary and calculate its distributions within the specimen is required. Therefore, an extension of the mesoscopic model reviewed in Section 4.2 *including thermomechanic coupling* represents a key result obtained within this thesis and is presented in this chapter.

Let us note that such an thermomechanical coupling has already been included in macroscopic models and mathematical results in the fully coupled case have been obtained as in e.g. (Krejčí and Stefanelli, 2011) for the Souza-Auricchio model (cf. (Auricchio and Petrini, 2004; Souza et al., 1998)) or in e.g. (Colli et al., 2000; Colli and Sprekels, 1992; Stefanelli, 2002, 2005) for the Frémond model (cf. (Frémond, 1987)).

This chapter is built up upon the works (Benešová and Roubíček, 2012; Benešová, 2011*b*), but also new results, not presented in these papers, are exposed in Section 5.5; also the proof Proposition 5.9 has not been presented elsewhere in full length.

Within this chapter, we first introduce the devised extension to thermally coupled case in Section 5.1; we also line out thermodynamic consistency in Section 5.2. Then, in Sections 5.4 and 5.5 we prove existence of solutions to thermally coupled model by two different methods, each of them having its own significance. The first method extends the ideas from Theorem 4.1 to show, that even in thermally coupled case the mesoscopic model can be understood as an approximations of microscopic models when the interfacial energy becomes negligible, i.e. the specimen becomes large. The second method, on discrete equivalent to the model and hence offers a conceptual numerical algorithm.

5.1 Presentation of the devised thermally coupled model

Since the model presented in this subsection aims to extend mesoscopic models as presented in Section 4.2, we again formulate the model within the framework of generalized standard solids in continuum mechanics and the large strain setting. Recall from Chapter 3 that this requires us to first find an appropriate set of internal variables, and further to prescribe *two potentials*, namely the Gibbs free energy and the dissipation potential to constitutively determine the behavior of the SMA specimen.

As to the set of state variables, we follow Section 4.2 and take $y \in W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^d)$, the averaged deformation, $\nu \in \mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^{d\times d})$, i.e. the gradient Young measure representing the microstructure due to very fine oscillations of the deformation gradient, and also the vector of volume fractions $\lambda \in \mathbb{R}^{M+1}$ as state variables. Furthermore, to capture thermal evolution, we enrich this set by the *temperature* $\theta \in \mathbb{R}$.

As to the choice of the Gibbs free energy, $\mathcal{G}$, we start from the form prescribed in the static case

$$\mathcal{G}^{\mathrm{S}}(y,\nu,\theta) = \int_\Omega \psi(\cdot,\theta)\bullet\nu - f\cdot y\,\mathrm{d}x - \int_{\Gamma_N} g\cdot y\,\mathrm{d}S;$$

however, we let the Helmholtz (and thus also the Gibbs) free energy depend also on the new state variable λ[1]. Moreover we consider, as quite usual (Falk, 1980; Falk and Konopka, 1990), the partially linearized ansatz

$$\tilde{\psi}_0(F,\lambda,\theta) = \underbrace{\phi_0(\theta)}_{\substack{\text{thermal}\\ \text{part}}} + \underbrace{\phi_1(F)}_{\substack{\text{multiwell}\\ \text{mechanical part}}} + \underbrace{(\theta-\theta_{\mathrm{tr}})\vec{a}\cdot\lambda}_{\substack{\text{thermomechanical}\\ \text{coupling}}}, \tag{5.1}$$

which restricts the assumptions from (4.2)[2]. Still, in (5.1), the multiwell mechanic part $\phi_1(F)$ can be chosen, for example, as in (4.5) with thermal part canceled in (4.6). Choosing $\phi_1(F)$ of a multiwell character will enable the formation of microstructure; on the other hand, simultaneously, the need for relaxation will arise as already in Chapter 4.

In the term corresponding to thermomechanic coupling $(\theta-\theta_{\mathrm{tr}})\vec{a}\cdot\lambda$ we set $\vec{a} = (0,\dots,0,-s_{\mathrm{tr}})$ where s_{tr} is the the specific transformation entropy, i.e. the difference of martensite versus austenite entropy, or, in other words, the latent heat of the martensitic transformation divided by the transformation temperature $\theta_{\mathrm{tr}} > 0$. Furthermore s_{tr} corresponds also, roughly, to the so-called *Clausius-Clapeyron constant* multiplied by a transformation strain, cf. (Arndt et al., 2006; Kružík et al., 2005). Furthermore, the chosen coupling term is the leading term in the *chemical energy* (Sedlák et al., 2012).

Note that an important feature of this ansatz is that the mechanic part entering thermomechanic coupling is representing *only* by the vector of volume factions; thus we implicitly *neglect thermal expansion*. Even though this approach is a simplification, the important feature that when temperature rises up, martensite takes higher energy than austenite becoming thus energetically preferable at higher temperatures, and vice versa for lower temperatures is captured through the coupling term; hence the *thermally induced martensitic transformation* can be modeled. Note that this simplified coupling will also be important from the mathematical point of view as mentioned in Remark 5.5.

[1] We shall denote the Helmholtz free energy depending on the variables (F,λ,θ) as $\tilde{\psi}_0 = \tilde{\psi}_0(F,\lambda,\theta)$ to distinguish it from the static free energy ψ depending only on (F,θ).

[2] Recall that in (4.2) we *only* required the Helmholtz free energy to be of a multiwell type with energetically preferable martensite wells for $\theta < \theta_{\mathrm{tr}}$ while for $\theta > \theta_{\mathrm{tr}}$ the austenite well takes the lowest energy.

5.1.1 Introducing a phase field

In Section 4.2 the vector of volume fractions λ was *fully determined* by the second mechanic variable ν through the relation (4.14); this approach was also used in (Kružík et al., 2005; Roubíček et al., 2007). In the macroscopic models, on the other hand, the volume fraction of martensite and the deformation gradient are regarded as completely independent (see e.g. (Frémond and Miyazaki, 1996; Sadjadpour and Bhattacharya, 2007*b*)).

Inspired by the macroscopic case, we choose, for thermally coupled model, a kind of a compromise approach: we still have λ and ν independent but we have in mind that, at least with some accuracy, $\lambda \sim L\bullet\nu$ with respect to a certain norm, denoted by $\mathcal{Q}_\varkappa(\cdot)^{1/2}$, rather than exactly having zero residuum $\lambda - L(F) = 0$. Hence, λ will correspond to a *phase field* that will enjoy higher regularity in time and that will be equal to the vector of volume fractions determined by the microstructure ν up to some small mismatch only.

The mentioned norm is considered as

$$\mathcal{Q}_\varkappa(\xi) = \int_\Omega \frac{\varkappa}{2}|\mathfrak{Q}\xi|^2 \,\mathrm{d}x \qquad \text{with some } \ \mathfrak{Q} \in \mathrm{Lin}(L^2(\Omega), L^2(\Omega)) \ \text{ compact,} \tag{5.2}$$

with $\varkappa$ presumably large. Note that the differential

$$\mathcal{Q}'_\varkappa(\xi) = \varkappa\mathfrak{Q}^*\mathfrak{Q} \in \mathrm{Lin}(L^2(\Omega), L^2(\Omega)) \tag{5.3}$$

is a compact operator, too. For an example, one can think of $\mathfrak{Q} = \nabla\Delta^{-1}$ and then simply $\mathcal{Q}'_\varkappa = -\varkappa\Delta^{-1}$; in this case $\mathcal{Q}_\varkappa(\cdot)^{1/2}$ is equivalent to the $H^{-1}(\Omega)$-norm as shown in (Benešová, Kružík and Roubíček, 2012).

For further shortening of notation let us introduce

$$\mathcal{P}_\varkappa(\nabla y, \lambda) = \mathcal{Q}'_\varkappa(\lambda - L(\nabla y)), \tag{5.4}$$

$$\mathcal{P}_\varkappa(\nu, \lambda) = \mathcal{Q}'_\varkappa(\lambda - L\bullet\nu). \tag{5.5}$$

To assure that $\lambda \sim L\bullet\nu$ with respect to the norm $\mathcal{Q}_\varkappa(\cdot)^{1/2}$, we augment the Gibbs free energy used in the static case, $\mathcal{G}^{\mathrm{S}}$, by the term $\mathcal{Q}_\varkappa(\lambda - L\bullet\nu)$, which results to

$$\mathcal{G}(t,y,\nu,\lambda,\theta) = \underbrace{\int_\Omega \widetilde{\psi}_0(\cdot,\lambda,\theta)\bullet\nu \,\mathrm{d}x}_{\text{stored energy}} + \underbrace{\mathcal{Q}_\varkappa(\lambda - L\bullet\nu)}_{\text{mismatch term}} - \underbrace{\int_\Omega f(t,\cdot)\cdot y \,\mathrm{d}x - \int_{\Gamma_{\mathrm{N}}} g(t,\cdot)\cdot y \,\mathrm{d}S}_{\text{energy of the applied load}}. \tag{5.6}$$

Remark 5.1 (Mathematical advantages of the phase field model). Implementing the phase field concept makes the model mathematically amenable. Indeed, if the holonomic constraint $\lambda = L\bullet\nu$ was required to be fulfilled this would lead to a strong coupling between the (rate-independent) evolution of ν and the (rate-dependent) evolution of the temperature θ. In turn, this would make it very hard to proove existence of solutions of thermally coupled model; in particular the flow-rule (5.11b) below would rather be a *doubly non-linear inclusion*.

Remark 5.2 (Justification of the phase-field approach). In order to justify the phase-field approach, let us prove that, under assumptions (A1), (A3) from Section 5.3, in the *static case* solutions $(\lambda_\varkappa, \nu_\varkappa)$ of the "penalized" problem[3]

$$\left.\begin{array}{ll} \text{minimize} & \displaystyle\int_\Omega \phi_1\bullet\nu + (\theta-\theta_{\mathrm{tr}})\vec{a}\cdot\lambda - \phi_0(\theta)\,\mathrm{d}x + \mathcal{Q}_\varkappa(\lambda - L\bullet\nu) \\ \text{subject to} & \nu \in \mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d}), \quad \lambda \in H_{\mathcal{Q}_\varkappa}(\Omega;\mathbb{R}^{M+1}) \quad \text{with } \theta \in C^1(\Omega)^4. \end{array}\right\} \tag{5.7}$$

[3]For simplicity, we omit the external forces here; however, they could be routinely included.

with $H_{\mathcal{Q}_\varkappa}(\Omega;\mathbb{R}^{M+1})$ the formal completion of the space of functions in $L^2(Q;\mathbb{R}^{M+1})$ equipped with the $\mathcal{Q}_\varkappa^{1/2}$-norm, converge in $H_{\mathcal{Q}_\varkappa}(\Omega;\mathbb{R}^{M+1})\times\mathscr{G}^p_{\Gamma_{\rm D}}(\Omega;\mathbb{R}^{d\times d})$ to solutions of

$$\left.\begin{array}{ll}\text{minimize} & \displaystyle\int_\Omega \phi_1\bullet\nu+(\theta-\theta_{\rm tr})\vec{a}\cdot\lambda-\phi_0(\theta)\,{\rm d}x\\ \text{subject to} & \nu\in\mathscr{G}^p_{\Gamma_{\rm D}}(\Omega;\mathbb{R}^{d\times d}),\quad \lambda\in H_{\mathcal{Q}_\varkappa}(\Omega;\mathbb{R}^{M+1})\quad\text{with }\theta\in C^1(\Omega).\\ & \text{and }\lambda=L\bullet\nu\text{ for a.a. }x\in\Omega.\end{array}\right\}\tag{5.8}$$

if $\varkappa\to\infty$.

Indeed, it easy to see, simply by testing (5.7) by any $(\hat\lambda,\hat\nu)$ such that $\hat\lambda=L\bullet\hat\nu$, that $\int_\Omega|\cdot|^p\bullet\nu_\varkappa\,{\rm d}x$ is bounded uniformly with respect to $\varkappa$.[5] Hence also $\|L\bullet\nu_\varkappa\|_{L^2(\Omega;\mathbb{R}^{d+1})}$[6] and in turn also $\mathcal{Q}_\varkappa(L\bullet\nu_\varkappa)$ are uniformly bounded with respect to $\varkappa$. By this test, we, furthermore, get that $\mathcal{Q}_\varkappa(\lambda_\varkappa-L\bullet\nu_\varkappa)$ and thus also $\|\lambda_\varkappa\|_{H_{\mathcal{Q}_\varkappa}(\Omega;\mathbb{R}^{M+1})}$ are bounded independently of $\varkappa$.

Thus, exploiting standard selection principles, we find a pair $(\lambda,\nu)\in H_{\mathcal{Q}_\varkappa}(\Omega;\mathbb{R}^{M+1})\times\mathscr{G}^p_{\Gamma_{\rm D}}(\Omega;\mathbb{R}^{d\times d})$ such that (in terms of a not-relabeled subsequence) $\nu_\varkappa\overset{*}{\rightharpoonup}\nu$ in $\mathscr{G}^p_{\Gamma_{\rm D}}(\Omega;\mathbb{R}^{d\times d})$ and $\lambda_\varkappa\rightharpoonup\lambda$ in $H_{\mathcal{Q}_\varkappa}(\Omega;\mathbb{R}^{M+1})$. Also, as $\mathcal{Q}_\varkappa(\lambda_\varkappa-L\bullet\nu_\varkappa)$ is bounded independently of $\varkappa$, necessarily $\lambda=L\bullet\nu$ holds for the weak limits.

Then thanks to the weak-lower semi-continuity we have that

$$\begin{aligned}\int_\Omega\phi_1\bullet\nu+(\theta-\theta_{\rm tr})\vec{a}\cdot\lambda-\phi_0(\theta)\,{\rm d}x&\le\liminf_{\varkappa\to\infty}\int_\Omega\phi_1\bullet\nu_\varkappa+(\theta-\theta_{\rm tr})\vec{a}\cdot\lambda_\varkappa-\phi_0(\theta)\,{\rm d}x\\&\le\liminf_{\varkappa\to\infty}\int_\Omega\phi_1\bullet\nu_\varkappa+(\theta-\theta_{\rm tr})\vec{a}\cdot\lambda_\varkappa-\phi_0(\theta)\,{\rm d}x+\mathcal{Q}_\varkappa(\lambda_\varkappa-L\bullet\nu_\varkappa)\\&\le\liminf_{\varkappa\to\infty}\int_\Omega\phi_1\bullet\hat\nu+(\theta-\theta_{\rm tr})\vec{a}\cdot\hat\lambda-\phi_0(\theta)\,{\rm d}x+\mathcal{Q}_\varkappa(\hat\lambda-L\bullet\hat\nu)\\&=\int_\Omega\phi_1\bullet\hat\nu+(\theta-\theta_{\rm tr})\vec{a}\cdot\hat\lambda-\phi_0(\theta)\,{\rm d}x,\end{aligned}$$

for any $(\hat\lambda,\hat\nu)$ such that $\hat\lambda=L\bullet\hat\nu$, which shows that (λ,ν) is a solution to (5.8).

Even though Remark 5.2 is concerned only with the static situation, a similar result can be proved also in the evolutionary but isothermal setting from Section 4.2; cf. (Benešová, Kružík and Roubíček, 2012) for details. We shall prove a result of this type also in thermally coupled, however *convex*, case in Chapter 6 below. Even though in the non-convex thermally coupled a result of this kind is still missing, the known results justify in a certain sense the mathematically favorable penalty approach.

5.1.2 Dissipation and heat equation

Following further the concept of generalized standard materials; we define the following dissipation potential

$$R(\dot\lambda)=\int_\Omega\rho_q(\dot\lambda)\,{\rm d}x\tag{5.9}$$

where

$$\rho_q(\xi)=\frac{\alpha}{q}|\xi|^q+\delta^*_S(\xi)\tag{5.10}$$

[5] Also, we have in mind the coercivity of ϕ_1 (i.e. (A1) from Section 5.3) – p then corresponds to (A1).

[6] We exploit assumption (A3) stating that $0\le L_i(\cdot)\le 1$ for $i=1\dots M+1$.

with $\alpha > 0$, $q \geq 2$ and $\delta_S^*(\cdot)$ the Legendre-Fenchel conjugate[7] *convex set* $S \subset \mathbb{R}^{M+1}$.

As to the interpretation of the terms in (5.9), $\delta_S^*(\xi)$ describes rate-independent losses (the contribution of which we consider dominant) and term $\frac{\alpha}{q}|\xi|^q$ models rate-dependent dissipation. As α is presumably small, our choice of the dissipation potential implies that at small rates (small driving forces) the behavior of the material is nearly rate-independent, but becomes rate-dependent at higher rates (large driving forces). It has been argued in (Sadjadpour and Bhattacharya, 2007*b*) that such a choice is necessary as "boundaries require an unboundedly increasing driving force for the propagation speeds to reach towards some sound speed", cf. also (Bhattacharya et al., 2003). This is also consistent with experiments, see again (Sadjadpour and Bhattacharya, 2007*b*) and the references therein. As was also noted in (Sadjadpour and Bhattacharya, 2007*b*) the *rate-dependents effect take place in a range of loading frequencies for which the isothermality assumption is mostly violated*; therefore it makes sense to include the rate-independent terms here even if they were omitted on Section 4.2. We include the rate-dependent term here, however, not only for its physical relevance but also for mathematical reasons which we expose in Remark 5.3.

Hence, in view of (3.17)-(3.19), we solve in $Q = [0,T] \times \Omega$ the following system

$$\partial_\nu \big(\mathcal{G}(t,y,\nu,\lambda,\theta) + \delta_{\mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^d)}(\nu) \big) \ni 0, \tag{5.11a}$$

$$\partial_{\dot\lambda} R(\dot\lambda) + \partial_\lambda \mathcal{G}(t,y,\nu,\lambda,\theta) \ni 0, \tag{5.11b}$$

$$\theta \dot s + \operatorname{div} j = \text{ heat-production rate} = \partial \rho_q(\dot\lambda) \cdot \dot\lambda, \tag{5.11c}$$

that is understood very formally, in particular the indicator function $\delta_{\mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^d)}(\nu)$ is not convex. We give a more suitable (and in fact even more restrictive) strong formulation reflecting the non-convexities in Section 5.1.3. Also, we did not specify the initial/boundary conditions and will do so again in Section 5.1.3.

At this point, let us, however, evaluate the entropy balance (5.11c). Due to the Gibbs relation $s = -[\tilde\psi_0(F,\lambda,\theta)]'_\theta(\lambda,\theta)$ (see also (3.9)), we have that $\dot s = -[\tilde\psi_0]''_{\theta\lambda}(\lambda,\theta)\cdot\dot\theta - [\tilde\psi_0]''_{\theta\lambda}\dot\lambda$ where $[\tilde\psi_0]''_{\theta\lambda} = \vec a$. This allows us to reformulate the entropy imbalance into a *heat equation*

$$c_{\rm v}(\theta)\dot\theta - \operatorname{div}(q) = \delta_S^*(\dot\lambda) + \alpha|\dot\lambda|^q + \vec a\cdot\theta\dot\lambda \quad \text{ with } \; c_{\rm v}(\theta) = -\theta[\tilde\psi_0]''_\theta(\theta), \tag{5.12}$$

where $c_{\rm v}$ is the specific *heat capacity*. In (5.12), the last term stems from *thermomechanic coupling* and is referred to as *adiabatic heat*. Furthermore, we have to make a constitutive choice for the heat-flux q; we consider it governed by the Fourier law

$$q = -\mathbb{K}(\lambda,\theta)\nabla\theta \tag{5.13}$$

[7] Recall, from Chapter 3, that for a function $f : \mathbb{R}^{M+1} \to \mathbb{R}$, we define its convex conjugate as (Rockafellar, 1970)

$$f^*(x^*) = \sup_{x\in\mathbb{R}^{M+1}} \{(x^*,x) - f(x)\}.$$

For example, consider the indicator function to the hypercuboid $\mathcal{C}_{\mathbb{R}^{M+1}} = \{x \in \mathbb{R}^{M+1}; |x_i| \leq \gamma_i\}$ for some $\gamma_i \geq 0$ given. Then, for its Legendre-Fenchel conjugate we have

$$\delta^*_{\mathcal{C}_{\mathbb{R}^{M+1}}}(x^*) = \sup_{x\in\mathbb{R}^{M+1}} \Big\{ (x^*,x) - \delta_{\mathcal{C}_{\mathbb{R}^{M+1}}}(x) \Big\} = \sup_{x\in\mathcal{C}_{\mathbb{R}^{M+1}}} \Big\{ \sum_{i=1}^{M+1} x_i^* x_i \Big\}.$$

In order to maximize this expression, we maximize each particular term of the sum $x_i^* x_i$. It is easy to see, that the maximum is obtained if choosing $x_i = \gamma_i x_i^*/|x_i^*|$ and hence

$$\delta^*_{\mathcal{C}_{\mathbb{R}^{M+1}}}(x^*) = \sum_{i=1}^{M+1} \gamma_i |x_i^*|.$$

Note that this form indeed corresponds to (4.15).

with $\mathbb{K}$ the *heat-conductivity* tensor. For thermodynamic consistency, we have to assume that $\mathbb{K}$ is *positive definite*; cf. assumption (A5) in Section 5.3 below where even a stricter ellipticity-like requirement is assumed.

Remark 5.3 (Mathematical reasons to consider a rate-dependent dissipation potential).

Mathematically, having a *rate-dependent dissipation potential* and $q \geq 2$ in (5.9) is essential due to the *adiabatic heat term* in (5.12). Indeed, if we neglected the rate-dependent contribution to the dissipation potential (by setting $\alpha = 0$ in (5.9)) one could expect at most $\dot{\lambda} \in L^1([0,T]; L^1(\Omega; \mathbb{R}^{M+1}))$. Thus, in order to have the adiabatic heat well defined, one would need to prove that $\theta \in L^\infty([0,T]; L^\infty(\Omega))$, which cannot be obtained due to the terms stemming from dissipation on the right-hand side of the heat equation (5.12).

5.1.3 Governing equations in strong form

In this subsection, let us give a suitable strong formulation of the very formal system (5.11). As already pointed out, especially (5.11a) is understood rather formally. Therefore, instead of (5.11a) we introduce the minimization problem (5.17a) – if the set of gradient Young measures and the Gibbs free energy were convex, (5.11a) and (5.17a) would be equivalent. In the non-convex case (5.17a) is even more restrictive but reflects the physically well accepted idea of (stored) energy minimization.

Further, it is mathematically advantageous to perform the so-called *enthalpy transformation* [8]. For this, let us introduce a new variable w, called *enthalpy*, by

$$w = \widehat{c}_{\rm v}(\theta) = \int_0^\theta c_{\rm v}(r)\,{\rm d}r. \tag{5.14}$$

It is natural to assume that $c_{\rm v}$ is positive, hence $\widehat{c}_{\rm v}$ is increasing and thus invertible[9]. Therefore, denote

$$\Theta(w) := \begin{cases} \widehat{c}_{\rm v}^{-1}(w) & \text{if } w \geq 0 \\ 0 & \text{if } w < 0 \end{cases} \tag{5.15}$$

and note that $\theta = \Theta(w)$. From the definition of w, we immediately see that $\dot{w} = c_{\rm v}(\theta)\dot{\theta}$. Rewriting further the heat flux in terms of w gives

$$\mathbb{K}(\lambda,\theta)\nabla\theta = \mathbb{K}\big(\lambda,\Theta(w)\big)\nabla\Theta(w) = \mathcal{K}(\lambda,w)\nabla w, \tag{5.16}$$

where $\mathcal{K}(\lambda,w) = \frac{\mathbb{K}(\lambda,\Theta(w))}{c_{\rm v}(\Theta(w))}$.

All in all, we end up with the following governing equations:

$$\left.\begin{aligned} \text{minimize}\quad & \int_\Omega \phi_1 \bullet \nu + \Theta(w)\lambda - f(t,\cdot)\cdot y\,{\rm d}x \\ & + \mathcal{Q}_\varkappa\big(\lambda - L\bullet\nu\big) - \int_{\Gamma_{\rm N}} g(t,\cdot)\cdot y\,{\rm d}S \\ \text{subject to}\quad & (y,\nu) \in W^{1,p}(\Omega;\mathbb{R}^d) \times \mathscr{G}^p_{\Gamma_{\rm D}}(\Omega;\mathbb{R}^{d\times d}) \\ & \text{such that } \nabla y = {\rm id}\bullet\nu \ \text{ and } (\lambda,\theta) \text{ are fixed,} \end{aligned}\right\} \quad \text{for } t\in[0,T], \tag{5.17a}$$

$$\partial\delta_S^*(\dot{\lambda}) + \alpha|\dot{\lambda}|^{q-2}\dot{\lambda} + (\Theta(w)-\theta_{\rm tr})\vec{a} \ni -\varkappa\mathfrak{D}^*\mathfrak{Q}(\lambda - L\bullet\nu) \qquad \text{in } Q, \tag{5.17b}$$

$$\dot{w} - {\rm div}(\mathcal{K}(\lambda,w)\nabla w) = \delta_S^*(\dot{\lambda}) + \alpha|\dot{\lambda}|^q + \Theta(w)\vec{a}\cdot\dot{\lambda} \qquad \text{in } Q, \tag{5.17c}$$

$$\big(\mathcal{K}(\lambda,w)\nabla w\big)\cdot n + b\Theta(w) = b\theta_{\rm ext} \qquad \text{on } \Sigma; \tag{5.17d}$$

[8] Introduced in the context of the so-called Stefan problem (Kamenomotskaya, 1961; Oleinik, 1960). Here we adapted it from (Roubíček, 2010).

[9] Here we assume that $\theta \geq 0$ since we understand θ to be the *absolute temperature*.

Note that (5.17b) was obtained from (5.11b) just by writing out the derivatives. Note further that we have added a Robin-type boundary condition for the heat equation in (5.17d) with $b > 0$ prescribed and $\theta_{\rm ext} > 0$ the given external temperature. The system (5.17) has thus to be completed by prescribing initial conditions in the form

$$y(0,\cdot) = y_0, \quad \nu(0,\cdot) = \nu_0, \quad \lambda(0,\cdot) = \lambda_0, \quad w(0,\cdot) = w_0 = \widehat{c}_{\rm v}(\theta_0) \qquad \text{on } \ \Omega, \quad (5.18)$$

that have to be compatible in the sense that $y_0 = {\rm id} \bullet \nu_0$ a.e. on $x \in \Omega$.

5.2 Thermodynamic consistency

Let us stress that the model proposed in this chapter with governing equations (5.17) is thermodynamically consistent, by which we understand that it *fulfills the first and the second law of thermodynamics*.

As to the second law, realize that the dissipation potential $R(\dot\lambda)$ is *convex* and the heat conduction tensor is assumed *positive definite* by (A5) in Section 5.3. In view of the discussion in Chapter 3, the second law of thermodynamics is satisfied, as desired.

It remains to show energy conservation. We show it for suitably smooth solutions $(y, \nu, \lambda, \theta)$ of (5.17); however instead of the enthalpy equation, we shall rather consider the original entropy balance (5.11c) with the heat flux governed by (5.13). Since (y, ν) minimize the Gibbs free energy $\mathcal{G}$ the partial derivatives with respect to these variables evaluated at each minimizer need to be zero. Hence we can write

$$\begin{aligned}\mathcal{G}(T,&y(T),\nu(T),\lambda(T),\theta(T)) = \mathcal{G}(0,y_0,\nu_0,\lambda_0,\theta_0)\\ &+\int_0^T \langle \mathcal{G}'_\lambda(\nu(t),\lambda(t),\theta(t)),\dot\lambda(t)\rangle + \mathcal{G}'_\theta(\lambda(t),\theta(t)),\dot\theta(t)\rangle + \mathcal{G}'_t(t,y(t))\,{\rm d}t, \qquad (5.19)\end{aligned}$$

when realizing that, due to the assumed form of the Gibbs free energy (5.6), the partial derivatives of $\mathcal{G}$ depend only on the indicated state variables.

Let us furthermore exploit the flow-rule (5.17b), multiply it by $\dot\lambda$ and integrate over Ω and $[0,T]$. This leads to the following equality [10]

$$\int_0^T\!\!\int_\Omega \alpha|\dot\lambda| + \delta_S^*(\dot\lambda)\,{\rm d}x\,{\rm d}t = -\int_0^T \langle \mathcal{G}'_\lambda(\nu(t),\lambda(t),\theta(t)),\dot\lambda(t)\rangle. \qquad (5.20)$$

Furthermore, multiplying (5.11c) by 1 and integrating over Ω and $[0,T]$ leads to

$$\int_0^T\!\!\int_\Omega \theta\dot s - {\rm div}(\mathbb{K}(\lambda,\theta)\nabla\theta) = \int_0^T\!\!\int_\Omega \delta_S^*(\dot\lambda) + \alpha|\dot\lambda|^q\,{\rm d}x\,{\rm d}t.$$

Exploiting the divergence theorem for ${\rm div}(\mathbb{K}(\lambda,\theta)\nabla\theta)$ and also boundary condition (5.17d)[11] allows us to write, using also the prescribed form of the Gibbs free energy (5.6) and the Gibbs relation (cf. e.g. 3.9),

$$\begin{aligned}\int_0^T \langle \mathcal{G}'_\theta(\lambda(t),\theta(t)),\dot\theta(t)\rangle &= \int_0^T\!\!\int_\Omega s\dot\theta = -\int_0^T \frac{\rm d}{{\rm d}t}\int_\Omega \theta s\,{\rm d}x\,{\rm d}t + \int_0^T\!\!\int_\Omega \dot s\theta\,{\rm d}x\,{\rm d}t\\ &= -\int_0^T \frac{\rm d}{{\rm d}t}\int_\Omega \theta s\,{\rm d}x\,{\rm d}t + \int_0^T\!\!\int_\Omega \delta_S^*(\dot\lambda)+\alpha|\dot\lambda|^q\,{\rm d}x\,{\rm d}t + \int_0^T\!\!\int_\Gamma b\theta_{\rm ext} - b\theta\,{\rm d}S\,{\rm d}t. \qquad (5.21)\end{aligned}$$

[10] Realize that, though $\partial\delta_S^*(\dot\lambda)$ is a set-valued mapping, $\partial\delta_S^*(\dot\lambda)\cdot\dot\lambda = \delta_S^*(\dot\lambda)$ is *single valued*.

[11] When reformulated in terms of temperature rather then the enthalpy, (5.17d) reads as

$$\big(\mathbb{K}(\lambda,\theta)\nabla\theta\big)\cdot n + b\theta = b\theta_{\rm ext} \qquad \text{on } \Gamma.$$

Therefore, plugging (5.20) and (5.21) into (5.19) leads to

$$\underbrace{\Big(\mathcal{G}(T)+\int_\Omega (\theta s)(T)\,\mathrm{d}x\Big)}_{\substack{\textit{final}\textit{internal}\\ \text{energy}}}-\underbrace{\Big(\mathcal{G}(0)+\int_\Omega (\theta s)(0)\,\mathrm{d}x\Big)}_{\substack{\textit{initial}\textit{internal}\\ \text{energy}}}=\underbrace{\int_0^T \mathcal{G}_t'(t,y(t))\,\mathrm{d}t}_{\substack{\text{power of}\\ \text{mechanical forces}}}+\underbrace{\int_0^T\int_\Gamma b\theta_{\mathrm{ext}}+b\theta\,\mathrm{d}S\,\mathrm{d}t}_{\substack{\text{power of}\\ \text{thermal forces}}},$$

where we introduced the shorthand notation

$$\begin{aligned}\mathcal{G}(T)&=\mathcal{G}(T,y(T),\nu(T),\lambda(T),\theta(T))\\ \mathcal{G}(0)&=\mathcal{G}(0,y_0,\nu_0,\lambda_0,\theta_0).\end{aligned}$$

Thus, we obtained energy conservation.

5.3 Weak formulation, data qualifications, main result

In this section we give an appropriate weak formulation of the strong system (5.17); in particular, we use the standard weak formulation for the inclusion (5.17b) (see e.g. (Roubíček, 2005)) and the standard very weak formulation of the enthalpy equation (5.17c).

Definition 5.4. We call the quadruple $(y,\nu,\lambda,w)\in B([0,T];W^{1,p}(\Omega;\mathbb{R}^d))\times(\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d}))^{[0,T]}\times W^{1,q}([0,T];L^q(\Omega))\times L^1([0,T];W^{1,1}(\Omega))$ such that $\nabla y(t)=\mathrm{id}\bullet\nu$ for all $t\in[0,T]$ a.e. on Ω and $y=x$ on Σ_{D}[12] a weak solution of (5.17) with initial condition (5.18) if it satisfies:

1. The **minimization principle**

$$\mathcal{G}(t,y(t),\nu(t),\lambda(t),\Theta(w(t)))\le\mathcal{G}(t,\tilde y,\tilde\nu,\lambda(t),\Theta(w(t))),\tag{5.22}$$

for any couple $(\tilde y,\tilde\nu)\in W^{1,p}(\Omega;\mathbb{R}^d)\times\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d})$ such that $\nabla\tilde y=\mathrm{id}\bullet\tilde\nu$ a.e. on Ω and all $t\in[0,T]$.

2. The **flow rule**

$$\int_Q\big(\Theta(w)-\theta_{\mathrm{tr}}\big)\vec a\cdot\big(v-\dot\lambda\big)+\rho_q(v)+\varkappa\mathfrak{Q}(\lambda-L\bullet\nu)\mathfrak{Q}(v-\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t\ge\int_Q\rho_q(\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t.\tag{5.23}$$

for any $v\in L^q(Q;\mathbb{R}^{M+1})$.

3. The **enthalpy equation**:

$$\begin{aligned}\int_Q\mathcal{K}(\lambda,w)\nabla w\cdot\nabla\zeta-w\dot\zeta\,\mathrm{d}x\,\mathrm{d}t+\int_\Sigma b\Theta(w)\zeta\,\mathrm{d}S\,\mathrm{d}t=\int_\Omega w_0\zeta(0)\,\mathrm{d}x+\int_\Sigma b\theta_{\mathrm{ext}}\zeta\,\mathrm{d}S\,\mathrm{d}t\\ +\int_Q\Big(\delta_S^*(\dot\lambda)+\alpha|\dot\lambda|^q+\Theta(w)\vec a\cdot\dot\lambda\Big)\zeta\,\mathrm{d}x\,\mathrm{d}t,\end{aligned}\tag{5.24}$$

for any $\zeta\in C^1(\bar Q)$ with $\zeta(T)=0$

4. The remaining **initial conditions** in (5.18):

$\nu(0,\cdot)=\nu_0$ and $\lambda(0,\cdot)=\lambda_0$ in Ω.

Remark 5.5 (Coupling between (5.22)-(5.24)). Note that, due to the proposed linearized ansatz of the Helmholtz free energy in (5.1) and by introducing the phase-field λ, (5.24) determining ν and (5.24) determining w are coupled only through the intermediate equation (5.23). The advantage of this is, roughly, that both variables for which only little regularity is assumed (i.e. ν and w) are not coupled *directly* but by means of λ which enjoys a higher regularity.

[12] Recall that $\Sigma_{\mathrm{D}}=[0,T]\times\Gamma_{\mathrm{D}}$.

Data qualifications:
Furthermore, let us summarize the data qualifications needed to prove existence of solutions:

(A1) *Mechanical part of the Helmholtz free energy*: $\phi_1 \in C(\mathbb{R}^{d\times d})$ and there exist $0 < c_1 \le c_2$, such that $c_1|\cdot|^p \le \phi_1(\cdot) \le c_2(1+|\cdot|^p)$, where $p \in [1, \frac{2d}{d-2})$ if $d > 2$, otherwise $p \in [1, \infty)$ arbitrary.

(A2) *Outer forces*: $f \in W^{1,\infty}([0,T]; L^{p^*}(\Omega;\mathbb{R}^d))$ and $g \in W^{1,\infty}([0,T]; L^{p^\sharp}(\Gamma_{\rm N},\mathbb{R}^d))$, where p corresponds to (A1).

(A3) *Phase distribution function*: $L \in C(\mathbb{R}^{d\times d};\mathbb{R}^{M+1})$ and $L(\cdot) \in \{s \in \mathbb{R}^{M+1}, 0 \le s_i \le 1 \text{ for all } i = 1\dots M{+}1, \sum_0^{M+1} s_i = 1\}$.

(A4) *Specific heat capacity*: $c_v \in C(\mathbb{R})$ and there exists a constants $\omega_1 \ge \omega \ge q'$, $q \ge 2$, and $c_1, c_2 > 0$ such that $c_1(1{+}\theta)^{\omega-1} \le c_v(\theta) \le c_2(1{+}\theta)^{\omega_1-1}$.

(A5) *Heat conduction tensor* $\mathcal{K} \in C(\mathbb{R}\times\mathbb{R}, \mathbb{R}^{d\times d})$ and there exist $C_K > 0$, $\kappa_0 > 0$ such that $\mathcal{K}(\lambda, w) \le C_K$ and $\chi^{\rm T}\mathcal{K}(\lambda,w)\chi \ge \kappa_0|\chi|^2$ for all $\lambda \in \mathbb{R}$, $w \in \mathbb{R}$ and $\chi \in \mathbb{R}^d$.

(A6) *Heat-transfer boundary condition* : $\theta_{\rm ext} \in L^1(\Sigma)$, $\theta_{\rm ext} \ge 0$, and $b \in L^\infty(\Sigma)$, $b \ge 0$.

(A7) *Initial conditions*:
$\nu_0 \in \mathscr{G}^p_{\Gamma_{\rm D}}(\Omega;\mathbb{R}^{d\times d})$, $\quad \lambda_0 \in L^q(\Omega)$, $\quad \theta_0 \ge 0$, $\quad \widehat{c}_{\rm v}(\theta_0) \in L^1(\Omega)$.

The requirement that $p \in [1, \frac{2d}{d-2})$ in (A1) will only be needed in Section 5.4 and even there could be avoided by using a different type of interfacial energy in (5.26). Yet, if $d = 3$, (A1) states that $p \in [1, 6]$, which can be satisfied if we chose (the mechanical part of) our stored energy of St. Venant - Kirchhoff type (4.6).

Note also that the growth condition in (A1) is not compatible with the non-interpenetration condition stating that $\phi_1(F) \to \infty$ whenever $\det(F) \to 0$. This is due to the fact that, as we stressed in Chapter 2, relaxation results by means of Young measures as in (Kinderlehrer and Pedregal, 1994; Pedregal, 1997) work *only* with functions having a growth as in (A1). Unfortunately, also the set $\mathscr{G}^{\infty,-\infty}(\Omega;\mathbb{R}^{d\times d})$ (see (2.33), Section 2.3.2) is insufficient in our situation, too.[13]

Note also that (A4) implies that (taking also the natural constraint $\theta > 0$ into account)

$$w = \int_0^\theta c_v(r)\,{\rm d}r \ge c_1\int_0^\theta (1{+}r)^{\omega-1}\,{\rm d}r \ge c_1((1{+}\theta)^\omega{-}1) = c_1((1{+}\Theta(w))^\omega{-}1).$$

Let us now concentrate on the mathematical analysis of the non-convex problem (5.17a), namely we shall concentrate on the proof that solutions to (5.17a) exist under assumptions (A1)-(A7). Indeed, we can formulate the following theorem:

Theorem 5.6. *Let (A1)-(A7) hold. Then at least one weak solution (y, ν, λ, w) to the problem (5.17) in accord with Definition 5.4 does exist. Moreover, some of these solutions satisfies also*[14]

$$w \in L^r([0,T]; W^{1,r}(\Omega)) \cap W^{1,1}(I; W^{1,\infty}(\Omega)^*) \qquad \text{with } 1 \le r < \frac{d{+}2}{d{+}1}. \tag{5.25}$$

[13] In order to use $\mathscr{G}^{\infty,-\infty}(\Omega;\mathbb{R}^{d\times d})$ for relaxation, one would need to assure that the gradients of the infimizing sequences of the unrelaxed potential are, for *a.a.* $x \in \Omega$, supported a compact set K *such that there exists yet another open set* K_δ *for which* $K \subset K_\delta$ *and the relaxed functional is finite on* K_δ. Thus, augmenting the free energy by the indicator function of any compact set would not open a possibility for relaxation.

[14] This additional quality thanks to the fine estimates as in (Boccardo et al., 1997; Boccardo and Galloët, 1989).

Within this chapter, we give two different proofs of Theorem 5.6, each of them of its own particular importance.

Namely, in Section 5.4 we prove Theorem 5.6 by formulating yet another *physically relevant model*, namely a *microscopic* model including the interfacial energy due to laminate formation as in (4.9). We then show that if this interfacial energy *becomes negligible*, as it is the case for large specimen, solutions to the microscopic model converge to (some) solutions of the proposed mesoscopic model (5.17); this corresponds to Proposition 4.1 where a similar conjecture was prooved in the static case. This method of proof *justifies* the proposed model.

The other proposed method of proof exploits the *Rothe method* and hence forms a *conceptual numerical algorithm*, at least after a spatial discretization has been performed. Indeed, we introduce in Section 5.5 a partition $0 = t_0 \leq t_1 \leq t_2 \ldots \leq t_N \leq T$ of the interval $[0, T]$ and define a *time-discretization* of (5.17); subsequently we prove that solutions of this time-discrete problem converge to (some) weak solutions of (5.17). This result will be essential for numerical implementation in Chapter 7, since it will allow us to design a justified discretization of our problem.

Let us now turn our attention to the particular proofs within the next two sections.

5.4 Proof Theorem 5.6 via approximation through microscopic models

Within this section, we prove Theorem 5.6 by approximating the original mesoscopic model by *microscopic models with vanishing interfacial energy*; note that this section in large parts follows (Benešová and Roubíček, 2012). Furthermore, in this section we give the proof Proposition 5.9 in full length while in has only been sketched in (Benešová and Roubíček, 2012).

5.4.1 Introducing an appropriate microscopic model

First of all, let us devise an appropriate *microscopic model*, again, the framework of *generalized standard solids*. Hence, we propose a Gibbs free energy $\mathcal{G}_\varepsilon$ in the form:

$$\begin{aligned}\mathcal{G}_\varepsilon(t, y, \lambda, \theta) = &\underbrace{\int_\Omega \tilde{\psi}_0(\nabla y, \lambda, \theta)\,\mathrm{d}x}_{\text{Helmholtz free energy}} + \underbrace{\int_\Omega \frac{\varepsilon}{2}|\nabla^2 y|^2\,\mathrm{d}x}_{\text{interfacial energy}} + \underbrace{\mathcal{Q}_\varkappa(\lambda - L(\nabla y))}_{\text{mismatch term}} \\ &\underbrace{- \int_\Omega f(t,\cdot)\cdot y\,\mathrm{d}x - \int_{\Gamma_N} g(t,\cdot)\cdot y\,\mathrm{d}S}_{\text{energy of the applied load}}.\end{aligned} \tag{5.26}$$

Notice, that this form corresponds to the static form proposed in (4.9); however, here we already made use of the phase field approach described in Subsection 5.1.1 – hence, the Helmholtz free energy depends on this phase-field λ and the mismatch term has been added. Recall also from Section 4.1 that, in this case, no relaxation is needed due to the compactifying effect of the interfacial energy. Again, we assume the partially linearized ansatz for the Helmholtz free energy (5.1).

Next, we have to prescribe the dissipation potential, i.e.

$$R_\varepsilon(\dot{\lambda}, \nabla\dot{y}) = \underbrace{\int_\Omega \frac{\alpha}{q}|\xi|^q + \delta_S^*(\xi)\,\mathrm{d}x}_{\substack{\text{Dissipation due to} \\ \text{transformation/reorientation}}} + \underbrace{\int_\Omega \varepsilon|\nabla\dot{y}|\,\mathrm{d}x}_{\substack{\text{Small dissipation} \\ \text{due to pinning effects}}}, \tag{5.27}$$

Here, the first part of the dissipation potential is the same as in (5.9) (and so we will occasionally use the abbreviation ρ_q from (5.10)), the second part is rather needed for mathematical reasons yielding more regularity of ∇y (cf. Remark 5.11 below) however can "really microscopically" be related with a wiggly energy landscape, invented in (Abeyaratne et al., 1996; James, 1996) and further rigorously analyzed for the 1-D case in (Mielke and Truskinovsky, 2012). Note that we will scale this term to 0 as $\varepsilon \to 0$.

Plugging (5.26)-(5.27) into the general equations (3.17)-(3.19) and using again the Fourier law for the heat flux, using the same type of boundary conditions for temperature as for the mesoscopic system (5.17) and, lastly, also performing the enthalpy transformation (cf. (5.14)) yields the following system in strong formulation:

$$-\mathrm{div}\varepsilon\mathrm{Dir}(\nabla\dot{y})-\mathrm{div}\phi_1'(\nabla y)+\varepsilon\mathrm{div}^2\nabla^2 y+\mathrm{div}\big(\mathcal{P}_\varkappa(\nabla y,\lambda)L'(\nabla y)\big)\ni f \quad \text{in } Q, \tag{5.28a}$$

$$y(t,x)=x \quad \text{in } \Sigma_{\mathrm{D}}, \tag{5.28b}$$

$$\Big(\varepsilon\mathrm{Dir}(\nabla\dot{y})+\phi_1'(\nabla y)-\mathcal{P}_\varkappa(\nabla y,\lambda)L'(\nabla y)-\varepsilon\mathrm{div}\,\nabla^2 y\Big)n + \varepsilon(\mathrm{div}_{\mathrm{S}}n)\nabla^2 y{:}(n\otimes n)-\varepsilon\mathrm{div}_{\mathrm{S}}(\nabla^2 y{\cdot}n)=g \quad \text{on } \Sigma_{\mathrm{N}}, \tag{5.28c}$$

$$\varepsilon\nabla^2 y{:}(n\otimes n)=0 \quad \text{on } \Sigma, \tag{5.28d}$$

$$\partial\delta_S^*(\dot{\lambda})+\alpha|\dot{\lambda}|^{q-2}\dot{\lambda}+\Theta(w){\cdot}\vec{a}\ni\theta_{\mathrm{tr}}{\cdot}\vec{a}-\mathcal{P}_\varkappa(\nabla y,\lambda) \quad \text{in } Q, \tag{5.28e}$$

$$\dot{w}-\mathrm{div}(\mathcal{K}(\lambda,w)\nabla w)=\delta_S^*(\dot{\lambda})+\alpha|\dot{\lambda}|^q+\varepsilon|\nabla\dot{y}|+\Theta(w)\vec{a}{\cdot}\dot{\lambda} \quad \text{in } Q, \tag{5.28f}$$

$$\big(\mathcal{K}(\lambda,w)\nabla w\big){\cdot}n+b\Theta(w)=b\theta_{\mathrm{ext}} \quad \text{on } \Sigma. \tag{5.28g}$$

where $\mathcal{P}_\varkappa(\nabla y,\lambda)$ was defined in (5.4), Dir is a sub-gradients of the convex, positively 1-homogenous potential $|\cdot|$, n denotes the unit outward normal to Γ, and $\mathrm{div}_{\mathrm{S}}=\mathrm{Tr}(\nabla_{\mathrm{S}})$, with $\mathrm{Tr}:\mathbb{R}^{(d-1)\times(d-1)}\to\mathbb{R}^{d-1}$ the usual matrix trace, denotes the $(d-1)$-dimensional "surface divergence" with the tangential derivative ∇_{S} defined as $\nabla_{\mathrm{S}}v=\nabla v-(\nabla v{\cdot}n)n$. Notice that, (5.28,a-d) correspond to (3.17) augmented also with boundary conditions.

While boundary condition (5.28b) is rather standard, the complicated forms of (5.28,c-d) are necessary due to the second gradient of y in the interfacial energy; this effect is well known in mechanics of complex (also called non-simple) continua; we refer to (Fried and Gurtin, 2006; Podio-Guidugli and Vergara Caffarelli, 1990; Toupin, 1962) for details.

Again, we complete the system (5.28) by the initial conditions

$$y(0,\cdot)=y_{0,\varepsilon},\qquad \lambda(0,\cdot)=\lambda_{0,\varepsilon},\qquad w(0,\cdot)=w_{0,\varepsilon}=\widehat{c}_{\mathrm{v}}(\theta^{0,\varepsilon}) \qquad \text{on } \Omega, \tag{5.29}$$

where $(y_{0,\varepsilon},\lambda_{0,\varepsilon})$ are the initial deformation and the phase field, while $\theta_{0,\varepsilon}$ is the initial temperature.

We now turn to devising a weak formulation for (5.28). While for the flow-rule (5.28e) and the enthalpy equation (5.28f), we use a rather standard approach, similarly as in Definition 5.4, the weak formulation for the inclusions/equations (5.28,a-d) is to a great extend inspired by the *energetic formulation* for rate-independent processes (see e.g. (Francfort and Mielke, 2006; Mielke and Theil, 2004)) and its generalization, given in e.g. (Roubíček, 2010), for problems that include both rate-independent and rate-dependent processes.

Then weak solutions to the microscopic model are defined as follows:

Definition 5.7. We shall call the triple $(y_\varepsilon,\lambda_\varepsilon,w_\varepsilon)\in L^\infty([0,T],W^{2,2}(\Omega;\mathbb{R}^d))\times W^{1,q}([0,T];L^q(\Omega;\mathbb{R}^{M+1}))\times L^1([0,T];W^{1,1}(\Omega))$ satisfying $y_\varepsilon\in\mathrm{BV}([0,T];W^{1,1}(\Omega;\mathbb{R}^d))$ and $y_\varepsilon(t,x)=x$ on Σ_{D} a weak solution of (5.28) with the initial condition (5.29) if it fulfills:

1. The **semi-stability**:

$$\mathcal{G}_\varepsilon(t,y_\varepsilon(t),\lambda_\varepsilon(t),\Theta(w_\varepsilon(t)))\le\mathcal{G}_\varepsilon(t,\tilde{y}_\varepsilon,\lambda_\varepsilon(t),\Theta(w_\varepsilon(t)))+\varepsilon\int_\Omega|\nabla y_\varepsilon(t)-\nabla\tilde{y}_\varepsilon|\,\mathrm{d}x \quad (5.30)$$

for any $\tilde{y}_\varepsilon\in W^{2,2}(\Omega;\mathbb{R}^d)$ such that $\tilde{y}_\varepsilon=x$ on $\Gamma_{\rm D}$ and all $t\in[0,T]$ with $\mathcal{G}_\varepsilon$ defined in (5.26).

2. The **mechanical energy equality**:

$$\begin{aligned}\mathfrak{G}_\varepsilon(T,y_\varepsilon(T),\lambda_\varepsilon(T))+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T])=\mathfrak{G}_\varepsilon(0,y_{0,\varepsilon},\lambda_{0,\varepsilon})\\+\int_0^T\langle[\mathfrak{G}_\varepsilon]'_\lambda(t,y_\varepsilon(t),\lambda_\varepsilon(t)),\dot{\lambda}_\varepsilon\rangle+[\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon(t),\lambda_\varepsilon(t))\,\mathrm{d}t,\end{aligned} \quad (5.31)$$

where $\mathfrak{G}_\varepsilon$ abbreviates the mechanical part of the microscopic energy, i.e.

$$\mathfrak{G}_\varepsilon(t,y,\lambda)=\int_\Omega\phi_1(\nabla y)+\frac{\varepsilon}{2}|\nabla^2 y|^2-f\cdot y\,\mathrm{d}x+\mathcal{Q}_\varkappa(\lambda-L(\nabla y))-\int_{\Gamma_{\rm N}}g\cdot y\,\mathrm{d}S; \quad (5.32)$$

where Var_f was defined in (4.23).

3. The **flow rule**: For any $v\in L^q(Q)$

$$\int_Q\big(\Theta(w_\varepsilon)-\theta_{\rm tr}\big)\vec{a}\cdot\big(v-\dot{\lambda}_\varepsilon\big)+\rho_q(v)+\mathcal{P}_\varkappa(\lambda_\varepsilon-L(\nabla y_\varepsilon))(v-\dot{\lambda}_\varepsilon)\,\mathrm{d}x\,\mathrm{d}t\ge\int_Q\rho_q(\dot{\lambda}_\varepsilon)\,\mathrm{d}x\,\mathrm{d}t. \quad (5.33)$$

4. The **enthalpy equation**: For any $\zeta\in C^1(\bar{Q})$ with $\zeta(T)=0$,

$$\begin{aligned}\int_Q\mathcal{K}(\lambda_\varepsilon,w_\varepsilon)\nabla w_\varepsilon\cdot\nabla\zeta-w_\varepsilon\dot{\zeta}\,\mathrm{d}x\,\mathrm{d}t+\int_\Sigma b\Theta(w_\varepsilon)\zeta\,\mathrm{d}S\,\mathrm{d}t=\int_\Omega w^{0,\varepsilon}\zeta(0)\,\mathrm{d}x+\int_\Sigma b\theta_{\rm ext}\zeta\,\mathrm{d}S\,\mathrm{d}t\\+\int_Q\Big(\delta_S^*(\dot{\lambda}_\varepsilon)+\alpha|\dot{\lambda}_\varepsilon|^q+\Theta(w_\varepsilon)\vec{a}\cdot\dot{\lambda}_\varepsilon\Big)\zeta\,\mathrm{d}x\,\mathrm{d}t+\varepsilon\int_{\bar{Q}}\zeta\,\mathcal{H}_\varepsilon(\,\mathrm{d}x\,\mathrm{d}t).\end{aligned} \quad (5.34)$$

here we denoted by $\mathcal{H}_\varepsilon\in\mathcal{M}(\bar{Q})$ the measure (=heat production rate by rate-independent dissipation) defined by prescribing its values on every closed set $A=[t_1,t_2]\times B$, where $B\subset\Omega$ is a Borel set as $\mathcal{H}_\varepsilon(A)=\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;B\times[t_1,t_2])$.

5. The **remaining initial conditions** in (5.29): $y(0,\cdot)=y^{0,\varepsilon}$ and $\lambda(0,\cdot)=\lambda^{0,\varepsilon}$ in Ω.

Remark 5.8 (Mechanic part of the Gibbs free energy in Definition 5.7). Notice, that we are entitled to consider in (5.31) only the mechanic part of the Gibbs free energy. This is due to the modeling approach, when introducing the phase field λ and the linearized ansatz (5.1), so that the deformation y and the enthalpy w are *not directly coupled*. If the deformation and the enthalpy were directly coupled, we would rather demand a conservation of the overall Gibbs free energy as in (Roubíček, 2010).

Note that the weak formulation obtained in Definition 5.7 is indeed selective as shown in (Benešová and Roubíček, 2012, Remark 4.3).

We now assure existence of microscopic solutions through Lemma 5.9; let us stress that in this section C as understood as a *generic constant independent of* ε.

5.4.2 Existence analysis for the microscopic model

Proposition 5.9 (Existence of solutions to the microscopic model)**.** *Let* (A1)-(A6) *hold and let*

$$y_{0,\varepsilon}\in W^{2,2}(\Omega;\mathbb{R}^d),\qquad\lambda_{0,\varepsilon}\in L^q(\Omega),\qquad\theta_{0,\varepsilon}\ge0,\quad\widehat{c}_{\rm v}(\theta_{0,\varepsilon})\in L^1(\Omega).$$

Then, for fixed ε*, at least one weak solution to* (5.28) *together with initial conditions* (5.29) *in accord with Definition* 5.7 *does exist. Moreover, a solution can be found that satisfies*

$$\left.\begin{aligned}&\sup_{t\in[0,T]}\|y_\varepsilon(t)\|_{W^{2,2}(\Omega;\mathbb{R}^d)}\le C\varepsilon^{-1/2},\\&\sup_{t\in[0,T]}\|y_\varepsilon(t)\|_{W^{1,p}(\Omega;\mathbb{R}^d)}\le C,\\&\|y_\varepsilon(t)\|_{\mathrm{BV}([0,T];W^{1,1}(\Omega;\mathbb{R}^d))}\le C\varepsilon^{-1},\end{aligned}\right\}\tag{5.35}$$

$$\|\dot\lambda_\varepsilon\|_{L^q(Q;\mathbb{R}^{M+1})}\le C,\tag{5.36}$$

$$\|w_\varepsilon\|_{L^\infty([0,T];L^1(\Omega))}\le C,\tag{5.37}$$

$$\|w_\varepsilon\|_{L^r([0,T];W^{1,r}(\Omega))}\le C(r)\ \text{ with any }\ 1\le r<\frac{d+2}{d+1},\tag{5.38}$$

$$\|\dot w_\varepsilon\|_{\mathcal{M}([0,T];W^{1,\infty}(\Omega)^*)}\le C.\tag{5.39}$$

Proof. The proof is performed by the *Rothe method* of time-discretization. For lucidity, let us divide the proof into several steps.

Step 1: Defining and proving existence of discrete weak solutions to (5.28)
Let us introduce a partition of the interval $[0,T]$ $0=t_0\le t_1\le t_2\ldots\le t_N=T$ such that $(t_i-t_{i-1})=\tau$ for all $i=1\ldots N$ and employ a semi-implicit method of *time-discretization* in such a way that it *decouples* the discrete equivalent of (5.30) and (5.33) from the discrete analogue of the enthalpy equation (5.34) in any particular time-step k by using the "retarded" values of w in (5.40a).

Hence, we shall call the triple $(y^k_{\varepsilon,\tau},\lambda^k_{\varepsilon,\tau},w^k_{\varepsilon,\tau})\in W^{2,2}(\Omega;\mathbb{R}^d)\times L^{2q}(\Omega;\mathbb{R}^{M+1})\times W^{1,2}(\Omega)$ the discrete weak solution of (5.28) with initial condition (5.29), if it fulfills:

1. The **minimization problem**:

$$\begin{aligned}&\text{Minimize }\mathcal{G}_\varepsilon(t_k,y,\lambda,\Theta(w^{k-1}_{\varepsilon,\tau}))+\int_\Omega\tau|\lambda|^{2q}+\varepsilon|\nabla y-\nabla y^{k-1}_{\varepsilon,\tau}|+\tau\rho_q\Big(\frac{\lambda-\lambda^{k-1}_{\varepsilon,\tau}}{\tau}\Big)\,\mathrm{d}x\\&\text{subject to }(y,\lambda)\in W^{2,2}(\Omega;\mathbb{R}^d)\times L^{2q}(\Omega;\mathbb{R}^{M+1})\text{ such that }y=x\text{ on }\Gamma_{\mathrm{D}}.\end{aligned}\tag{5.40a}$$

2. The **enthalpy equation**: For all $\varphi\in W^{1,2}(\Omega)$ it holds

$$\begin{aligned}\int_\Omega\frac{w^k_{\varepsilon,\tau}-w^{k-1}_{\varepsilon,\tau}}{\tau}\varphi+\mathcal{K}(\lambda^k_{\varepsilon,\tau},w^k_{\varepsilon,\tau})\nabla w^k_{\varepsilon,\tau}\nabla\varphi\,\mathrm{d}x+\int_\Gamma b^k_\tau\Theta(w^k_{\varepsilon,\tau})\varphi\,\mathrm{d}S=\int_\Gamma\theta^k_{\mathrm{ext},\tau}\varphi\,\mathrm{d}S\\+\int_\Omega\varrho_q\Big(\frac{\lambda^k_{\varepsilon,\tau}-\lambda^{k-1}_{\varepsilon,\tau}}{\tau}\Big)\varphi+\left|\frac{y^k_{\varepsilon,\tau}-y^{k-1}_{\varepsilon,\tau}}{\tau}\right|\varphi+\Theta(w^k_{\varepsilon,\tau})\vec a\cdot\Big(\frac{\lambda^k_{\varepsilon,\tau}-\lambda^{k-1}_{\varepsilon,\tau}}{\tau}\Big)\varphi\,\mathrm{d}x,\end{aligned}\tag{5.40b}$$

where we abbreviated

$$\varrho_q(\xi)=\delta^*_S(\xi)+\alpha|\xi|^q.\tag{5.40c}$$

3. The **initial condition** in the sense that

$$y^0_{\varepsilon,\tau}=y_{0,\varepsilon}\qquad\lambda^0_{\varepsilon,\tau}=\lambda_{0,\varepsilon,\tau}\qquad\Theta(w^0_{\varepsilon,\tau})=\theta_{0,\varepsilon,\tau}\text{ for a.a. }x\in\Omega.\tag{5.40d}$$

In (5.40d), we denoted by $\lambda_{0,\varepsilon,\tau}\in L^{2q}(\Omega;\mathbb{R}^{M+1})$ a suitable approximation of the original initial condition $\lambda_{0,\varepsilon}\in L^q(\Omega;\mathbb{R}^{M+1})$, such that

$$\lambda_{0,\varepsilon,\tau}\to\lambda_{0,\varepsilon}\text{ strongly in }L^q(\Omega;\mathbb{R}^{M+1})\text{ and }\|\lambda_{0,\varepsilon,\tau}\|_{L^{2q}(\Omega;\mathbb{R}^{M+1})}\le C\tau^{-1/(2q+1)},\tag{5.41}$$

and by $\theta_{0,\varepsilon,\tau}$ an approximation of $\theta_{0,\varepsilon}$, such that $w^0_{\varepsilon,\tau}\in W^{1,2}(\Omega)$ and $\Theta(w^0_{\varepsilon,\tau})\to\theta_{0,\varepsilon}$ in $L^1(\Omega)$. Moreover $\theta^k_{\mathrm{ext},\tau}\in L^2(\Gamma)$ and $b^k_\tau\in L^\infty(\Gamma)$ are defined in such a way that their piecewise constant interpolants

$$[\bar\theta_{\mathrm{ext},\tau},\bar b_{\varepsilon,\tau}](t)=\big(\theta^k_{\mathrm{ext},\tau},b^k_\tau,\big)\qquad\text{for }\ (k-1)\tau<t\le k\tau,\ \ k=1,...,N.$$

satisfy

$$\bar{\theta}_{\mathrm{ext},\tau} \to \theta_{\mathrm{ext}} \text{ strongly in } L^1(\Sigma) \text{ and } \bar{b}_\tau \overset{*}{\rightharpoonup} b \text{ weakly* in } L^\infty(\Sigma). \tag{5.42}$$

To show existence of (5.40), we first note that (5.40a) and (5.40b) are decoupled; hence, we are entitled to first show existence of solutions to (5.40a) independently of (5.40b). To do so, we proceed by the direct method, i.e. take an infimizing sequence $\{q^{k,j}\}_{j=0}^\infty = \{y_{\varepsilon,\tau}^{k,j}, \lambda_{\varepsilon,\tau}^{k,j}\}_{j=0}^\infty$ of (5.40a). Then, due to the coercivity of the cost function through the surface energy term $\int_\Omega \varepsilon|\nabla^2 y_{\varepsilon,\tau}^{k,j}|^2 \,\mathrm{d}x$ and the regularization term $\int_\Omega \tau|\lambda_{\varepsilon,\tau}^{k,j}|^{2q} \,\mathrm{d}x$, $q^{k,j}$ is, for τ, ε fixed, bounded in $W^{2,2}(\Omega,\mathbb{R}^d) \times L^{2q}(\Omega;\mathbb{R}^{M+1})$; thus, we may extract a subsequence that converges weakly in this space some q^k. In addition, owing to assumption (A1), $y_{\varepsilon,\tau}^{k,j} \to y_{\varepsilon,\tau}^k$ *strongly* in $W^{1,p}(\Omega;\mathbb{R}^d)$. Hence, by convexity of cost function from (5.40a) in λ as well as in the second gradient of y, and by exploiting the above mentioned strong convergence of $y_{\varepsilon,\tau}^{k,j}$, q^k is the sought minimizer at time-step k.

The existence of solutions to (5.40b) for $k = 1$ (and subsequently also for all other k) can be proved by exploiting the Brezis' theorem (Roubíček, 2005). For this, note that due to the regularization term $|\lambda|^{2q}$ the right-hand side of the discrete enthalpy equation is an element of $W^{1,2}(\Omega)^*$.

Further, we assure that $w_{\varepsilon,\tau}^k$ are non-negative. To this end, let us test (5.40b) by $[w_{\varepsilon,\tau}^k]^- \equiv \min(0, w_{\varepsilon,\tau}^k)$ (which is a legal test function as $w_{\varepsilon,\tau}^k \in W^{1,2}(\Omega)$). We get

$$\int_\Omega w_{\varepsilon,\tau}^k[w_{\varepsilon,\tau}^k]^- + \tau\mathcal{K}(\lambda_{\varepsilon,\tau}^k, w_{\varepsilon,\tau}^k)\nabla w_{\varepsilon,\tau}^k \nabla[w_{\varepsilon,\tau}^k]^- \,\mathrm{d}x \le \int_\Omega \tau\varrho_q\Big(\frac{\lambda_{\varepsilon,\tau}^k - \lambda_{\varepsilon,\tau}^{k-1}}{\tau}\Big)[w_{\varepsilon,\tau}^k]^- \,\mathrm{d}x$$
$$+ \int_\Omega \Theta(w_{\varepsilon,\tau}^k)\vec{a}\cdot(\lambda_{\varepsilon,\tau}^k - \lambda_{\varepsilon,\tau}^{k-1})[w_{\varepsilon,\tau}^k]^- + w_{\varepsilon,\tau}^{k-1}[w_{\varepsilon,\tau}^k]^- \,\mathrm{d}x - \tau\int_\Gamma b_\tau^k\Theta(w_{\varepsilon,\tau}^k)[w_{\varepsilon,\tau}^k]^- + \theta_{\mathrm{ext}}[w_{\varepsilon,\tau}^k]^- \,\mathrm{d}S$$

As $\Theta(w_{\varepsilon,\tau}^k)[w_{\varepsilon,\tau}^k]^- = 0$ (recall that we defined in (5.15) $\Theta(w) = 0$ for $w \le 0$) and also $\varrho_q\big(\frac{\lambda_{\varepsilon,\tau}^k - \lambda_{\varepsilon,\tau}^{k-1}}{\tau}\big) \ge 0$ and hence $\varrho_q\big(\frac{\lambda_{\varepsilon,\tau}^k - \lambda_{\varepsilon,\tau}^{k-1}}{\tau}\big)[w_{\varepsilon,\tau}^k]^- \le 0$ we get, when exploiting furthermore that $\theta_{\mathrm{ext}}[w_{\varepsilon,\tau}^k]^- \le 0$, that

$$\int_\Omega |[w_{\varepsilon,\tau}^k]^-|^2 + \tau\kappa_0|\nabla[w_{\varepsilon,\tau}^k]^-|^2 \,\mathrm{d}x \le \int_\Omega w_{\varepsilon,\tau}^{k-1}[w_{\varepsilon,\tau}^k]^- \,\mathrm{d}x.$$

When using this equation recursively and when also taking into account that $w_{\varepsilon,\tau}^0 \ge 0$ we get truly that $w_{\varepsilon,\tau}^k \ge 0$.

Step 2: Definition of interpolants and a-priori estimates
We introduce the notion of *piecewise affine* interpolants $y_{\varepsilon,\tau}$, $\lambda_{\varepsilon,\tau}$ and $w_{\varepsilon,\tau}$ defined by

$$\big[y_{\varepsilon,\tau}, \lambda_{\varepsilon,\tau}, w_{\varepsilon,\tau}\big](t) = \frac{t-(k-1)\tau}{\tau}\big(y_{\varepsilon,\tau}^k, \lambda_{\varepsilon,\tau}^k, w_{\varepsilon,\tau}^k\big) + \frac{k\tau - t}{\tau}\big(y_{\varepsilon,\tau}^{k-1}, \lambda_{\varepsilon,\tau}^{k-1}, w_{\varepsilon,\tau}^{k-1}\big), \tag{5.43}$$

for $t \in [(k-1)\tau, k\tau]$ with $k = 1, ..., T/\tau$.

In addition, we define the backward *piecewise constant interpolants* $\bar{\nu}_{\varepsilon,\tau}$, $\bar{\lambda}_{\varepsilon,\tau}$, and $\bar{w}_{\varepsilon,\tau}$ by

$$\big[\bar{y}_{\varepsilon,\tau}, \bar{\lambda}_{\varepsilon,\tau}, \bar{w}_{\varepsilon,\tau}\big](t) = \big(y_{\varepsilon,\tau}^k, \lambda_{\varepsilon,\tau}^k, w_{\varepsilon,\tau}^k\big) \qquad \text{for } (k-1)\tau < t \le k\tau, \ \ k = 1, ..., N. \tag{5.44}$$

Finally, define the "retarded" enthalpy piecewise constant interpolant $\underline{w}_{\varepsilon,\tau}$

$$[\underline{w}_{\varepsilon,\tau}(t)] = [w_{\varepsilon,\tau}^{k-1}] \qquad \text{for } (k-1)\tau < t \le k\tau, \ \ k = 1, ..., N. \tag{5.45}$$

For these interpolants we obtain a-priori estimates formulated in Lemma 5.10 (below) and proved, for the sake of clarity, following the current proof.

Lemma 5.10. *Let* (A1)-(A6) *hold and let*

$$y_{0,\varepsilon} \in W^{2,2}(\Omega;\mathbb{R}^d), \qquad \lambda_{0,\varepsilon} \in L^q(\Omega), \qquad \theta_{0,\varepsilon} \geq 0, \quad \widehat{c}_{\rm v}(\theta_{0,\varepsilon}) \in L^1(\Omega).$$

Then the piecewise affine interpolants $(y_{\varepsilon,\tau}, \lambda_{\varepsilon,\tau}, w_{\varepsilon,\tau})$ *defined through* (5.43) *and the piecewise constant interpolants* $(\bar{y}_{\varepsilon,\tau}, \bar{\lambda}_{\varepsilon,\tau}, \bar{w}_{\varepsilon,\tau})$ *defined through* (5.44) *satisfy*

$$\left.\begin{array}{l} \sup_{t\in[0,T]} \|\bar{y}_{\varepsilon,\tau}(t)\|_{W^{2,2}(\Omega;\mathbb{R}^d)} \leq C\varepsilon^{-1/2} \\ \sup_{t\in[0,T]} \|\bar{y}_{\varepsilon,\tau}(t)\|_{W^{1,p}(\Omega;\mathbb{R}^d)} \leq C \\ \|\bar{y}_{\varepsilon,\tau}(t)\|_{{\rm BV}([0,T];W^{1,1}(\Omega;\mathbb{R}^d))} \leq C\varepsilon^{-1} \end{array}\right\} \tag{5.46}$$

$$\|\dot{\bar{\lambda}}_{\varepsilon,\tau}\|_{L^q(Q;\mathbb{R}^{M+1})} \leq C, \tag{5.47}$$

$$\|\bar{\lambda}_{\varepsilon,\tau}\|_{L^\infty([0,T];L^{2q}(\Omega;\mathbb{R}^{M+1}))} \leq C\tau^{-1/2q} \tag{5.48}$$

$$\|\bar{w}_{\varepsilon,\tau}\|_{L^\infty([0,T];L^1(\Omega))} \leq C, \tag{5.49}$$

$$\|\bar{w}_{\varepsilon,\tau}\|_{L^r([0,T];W^{1,r}(\Omega))} \leq C(r) \text{ with any } 1 \leq r < \frac{d+2}{d+1}, \tag{5.50}$$

$$\|\dot{\bar{w}}_{\varepsilon,\tau}\|_{\mathcal{M}([0,T];W^{1,\infty}(\Omega)^*)} \leq C, \tag{5.51}$$

for some generic C *independent of* τ *and* ε.

Step 3: Selection of subsequences
By the a-priori estimates from Lemma 5.10, we may find a subsequence of τ's (not relabeled) and $(y_\varepsilon, \lambda_\varepsilon, w_\varepsilon)$ such that

$$\bar{y}_{\varepsilon,\tau}(t) \rightharpoonup y_\varepsilon(t) \quad \forall t \in [0,T] \text{ in } W^{2,2}(\Omega;\mathbb{R}^d) \tag{5.52}$$

$$\bar{\lambda}_{\varepsilon,\tau} \overset{*}{\rightharpoonup} \lambda_\varepsilon \quad \text{in } L^\infty([0,T];L^q(\Omega;\mathbb{R}^{M+1})) \tag{5.53}$$

$$\bar{\lambda}_{\varepsilon,\tau}(t) \rightharpoonup \lambda(t) \quad \forall t \in [0,T] \text{ in } L^q(\Omega;\mathbb{R}^{M+1}), \tag{5.54}$$

$$\dot{\bar{\lambda}}_{\varepsilon,\tau} \rightharpoonup \dot{\lambda}_\varepsilon \quad \text{in } L^q(Q;\mathbb{R}^{M+1}), \tag{5.55}$$

$$\bar{w}_{\varepsilon,\tau} \rightharpoonup w_\varepsilon \quad \text{in } L^r([0,T];W^{1,r}(\Omega)),\ r < \tfrac{d+2}{d+1} \text{ and } \bar{w}_{\varepsilon,\tau} \to w \text{ in } L^1(Q), \tag{5.56}$$

Indeed, by (5.47) we know that $\dot{\bar{\lambda}}_{\varepsilon,\tau}$ is bounded in $L^q(Q;\mathbb{R}^{M+1})$ and hence also $\bar{\lambda}_{\varepsilon,\tau}$ (considering also (5.41) and $\lambda_{0,\varepsilon} \in L^q(\Omega;\mathbb{R}^{M+1})$) is bounded in $L^\infty([0,T];L^q(\Omega;\mathbb{R}^{M+1}))$. Hence, by standard selection principles, we find λ_ε such that $\dot{\bar{\lambda}}_{\varepsilon,\tau} \rightharpoonup \dot{\lambda}_\varepsilon$ in $L^q(Q;\mathbb{R}^{M+1})$ and $\bar{\lambda}_{\varepsilon,\tau} \overset{*}{\rightharpoonup} \lambda_\varepsilon$ in $L^\infty([0,T];L^q(\Omega;\mathbb{R}^{M+1}))$.[15]

As $W^{1,q}(I;L^q(\Omega;\mathbb{R}^{M+1})) \subset C([0,T];L^q(\Omega;\mathbb{R}^{M+1}))$, we also get that $\bar{\lambda}_{\varepsilon,\tau}(t) \rightharpoonup \lambda_\varepsilon(t)$ for all $t \in [0,T]$ in $L^q(\Omega)$, i.e. (5.54).

As to $\bar{y}_{\varepsilon,\tau}$, we exploit (a slight) modification of the Helly's theorem (Mielke, 2005; Mielke et al., 2008) to find a y_ε in ${\rm BV}([0,T];W^{1,1}(\Omega,\mathbb{R}^d))$ such that $\bar{y}_{\varepsilon,\tau}(t) \rightharpoonup y_\varepsilon(t)$ in $W^{2,2}(\Omega,\mathbb{R}^d)$ for all $t \in [0,T]$.

Now, $\bar{w}_{\varepsilon,\tau}$ converges weakly to some w_ε in $L^r([0,T];W^{1,r}(\Omega))$, $r < \frac{d+2}{d+1}$ owing to the bound (5.50). Having the dual estimate on the time derivative of $w_{\varepsilon,\tau}$, *i.e.* (5.51), at our disposal, we exploit the Aubin-Lions-lemma generalized for measure-valued derivatives (see (Roubíček, 2005, Corollary 7.9)) to get that $\bar{w}_{\varepsilon,\tau}$ converges *even strongly* to w_ε in $L^{\frac{d+2}{d}-\delta}(Q)$; for any small $\delta > 0$ – cf. (Roubíček, 2010, Formulae (4.42) and (4.55)). Moreover the estimate (5.51) assures that the retarded enthalpy $\underline{w}_{\varepsilon,\tau}(t)$ converges strongly in $L^{\frac{d+2}{d}-\delta}(Q)$ *to the same limit* as $\bar{w}_{\varepsilon,\tau}$.

Thanks to the growth condition in assumption (A4), $|\Theta(w)| \leq C(1+|w|^{1/\omega}) \leq C(1+|w|^{1/q'})$.; thus we may apply the *Nemytskii theorem for mapping in Lebesgue*

[15] Note that, owing to (5.47), both $\lambda_{\varepsilon,\tau}$ and $\bar{\lambda}_{\varepsilon,\tau}$ converge weakly in $L^\infty([0,T];L^q(\Omega;\mathbb{R}^{M+1}))$ to the same limit because $\|\lambda_{\varepsilon,\tau} - \bar{\lambda}_{\varepsilon,\tau}\|_{L^q(Q;\mathbb{R}^{M+1})} \leq \tau \|\dot{\bar{\lambda}}_{\varepsilon,\tau}\|_{L^q(Q;\mathbb{R}^{M+1})}$

spaces (see e.g. (Roubíček, 2005)), using continuity of $\Theta(\cdot)$, to get that $\Theta(\bar{w}_{\varepsilon,\tau}) \to \Theta(w_\varepsilon)$ in $L^{q'}(Q)$. Similarly also $\Theta(\underline{w}_{\varepsilon,\tau}) \to \Theta(w_\varepsilon)$.

Finally, let us note that, relying on the lower semi-continuity of norms, the limits satisfy the bounds (5.35)–(5.39) with some C *independent of* ε.

Step 4: Convergence in the minimization principle and flow-rule
Let us fix, for the moment, some arbitrary $t \in [0,T]$. From (5.40a) we have the following *discrete minimization principle*

$$\mathfrak{G}_\varepsilon(t_\tau, \bar{y}_{\varepsilon,\tau}(t), \bar{\lambda}_{\varepsilon,\tau}(t)) \le \mathfrak{G}_\varepsilon(t_\tau, \hat{y}_\varepsilon, \bar{\lambda}_{\varepsilon,\tau}(t)) + \varepsilon \int_\Omega |\nabla \bar{y}_{\varepsilon,\tau} - \nabla \hat{y}_\varepsilon| \,\mathrm{d}x, \tag{5.57}$$

for any $\tilde{y}_\varepsilon \in W^{2,2}(\Omega;\mathbb{R}^d)$ such that $\tilde{y}_\varepsilon = x$ on Γ_{D}. In (5.57) we, furthermore, denoted $t_\tau = l\cdot\tau$, where $l = \min_{s\in\mathbb{N}}\{t \le s\tau\}$.

Let us exploit that $\bar{y}_{\varepsilon,\tau}(t) \rightharpoonup y_\varepsilon(t)$ weakly in $W^{2,2}(\Omega;\mathbb{R}^d)$ and hence, due to (A1), strongly in $W^{1,p}(\Omega;\mathbb{R}^d)$; thus, it follows that $\phi_1(\nabla\bar{y}_{\varepsilon,\tau}(t)) \to \phi_1(\nabla\bar{y}_\varepsilon(t))$ in $L^1(\Omega)$. Also, $L(\nabla\bar{y}_{\varepsilon,\tau}(t)) \to L(\nabla y_\varepsilon(t))$ in any $L^s(\Omega;\mathbb{R}^{M+1})$, $s \in [1,\infty)$ because $|L|$ is bounded by 1 (cf. (A3)). Further, since $\bar{\lambda}_{\varepsilon,\tau}(t) \rightharpoonup \lambda_\varepsilon(t)$ in $L^2(\Omega;\mathbb{R}^{M+1})$, also $\mathcal{Q}_\varkappa(\bar{\lambda}_{\varepsilon,\tau}(t) - L(\nabla\bar{y}_{\varepsilon,\tau}(t))) \to \mathcal{Q}_\varkappa(lambda_\varepsilon(t) - L(\nabla y_\varepsilon(t)))$ owing to the definition of $\mathcal{Q}_\varkappa$ in (5.2). Finally, by exploiting convexity of $\varepsilon|\nabla^2\bar{y}_{\varepsilon,\tau}(t)|^2$, we get by applying $\liminf_{\tau\to0}$ in (5.57)

$$\begin{aligned}
&\mathfrak{G}_\varepsilon(t, y_\varepsilon(t), \lambda_\varepsilon(t)) \le \liminf_{\tau\to0} \mathfrak{G}_\varepsilon(t_\tau, \bar{y}_{\varepsilon,\tau}(t), \bar{\lambda}_{\varepsilon,\tau}(t)) \le \limsup_{\tau\to0} \mathfrak{G}_\varepsilon(t_\tau, \bar{y}_{\varepsilon,\tau}(t), \bar{\lambda}_{\varepsilon,\tau}(t)) \\
&\le \limsup_{\tau\to0} \mathfrak{G}_\varepsilon(t_\tau, \hat{y}_\varepsilon, \bar{\lambda}_{\varepsilon,\tau}(t)) + \varepsilon \int_\Omega |\nabla\bar{y}_{\varepsilon,\tau} - \nabla\hat{y}_\varepsilon| \,\mathrm{d}x \le \mathfrak{G}_\varepsilon(t, \hat{y}_\varepsilon, \lambda_\varepsilon(t)) + \varepsilon \int_\Omega |\nabla y_\varepsilon - \nabla\hat{y}_\varepsilon| \,\mathrm{d}x,
\end{aligned}$$

where we exploited that $\mathcal{Q}_\varkappa(\bar{\lambda}_{\varepsilon,\tau}(t) - L(\nabla\hat{y}_\varepsilon)) \to \mathcal{Q}_\varkappa(lambda_\varepsilon(t) - L(\nabla\hat{y}_\varepsilon))$; hence, we established (5.30). In particular, we got that $\mathfrak{G}_\varepsilon(t_\tau, \bar{y}_{\varepsilon,\tau}(t), \bar{\lambda}_{\varepsilon,\tau}(t)) \to \mathfrak{G}_\varepsilon(t, y_\varepsilon(t), \lambda_\varepsilon(t))$ for all $t \in [0,T]$.

From now on, we do not fix t anymore and deduce the discrete flow rule by realizing that any subdifferential of the cost function in (5.40a) with respect to λ evaluated at $\bar{\lambda}_{\varepsilon,\tau}(t_j)$ (for some $j \in 1\dots N$) is equal to 0 and by summing these conditions from to 1 to N:

$$\begin{aligned}
\int_0^T\!\!\int_\Omega \rho_q(\dot{\lambda}_{\varepsilon,\tau}) \,\mathrm{d}x\,\mathrm{d}t \le \int_0^T\!\!\int_\Omega \mathcal{Q}'_\varkappa\big(\bar{\lambda}_{\varepsilon,\tau} - L(\nabla\bar{y}_{\varepsilon,\tau})\big)\cdot(v_{\varepsilon,\tau} - \dot{\lambda}_{\varepsilon,\tau}) + \rho_q(v_{\varepsilon,\tau}) \,\mathrm{d}x\,\mathrm{d}t \\
+ \int_0^T\!\!\int_\Omega (\Theta(\underline{w}_{\varepsilon,\tau}(t)) - \theta_{\mathrm{tr}})\vec{a}\cdot(v_{\varepsilon,\tau} - \dot{\lambda}_{\varepsilon,\tau}) + 2q\tau|\bar{\lambda}_{\varepsilon,\tau}|^{2q-2}\bar{\lambda}_{\varepsilon,\tau}(v_{\varepsilon,\tau} - \dot{\lambda}_{\varepsilon,\tau}) \,\mathrm{d}x\,\mathrm{d}t,.
\end{aligned} \tag{5.58}$$

for any $v_{\varepsilon,\tau}$ such that $v_\tau(\cdot,x)$ is piecewise constant on the intervals $(t_{j-1}, t_j]$ and $v_\tau(t_j,\cdot) \in L^{2q}(\Omega;\mathbb{R}^{d+1})$ for every j.

Now, let us choose some arbitrary test function $v_\varepsilon \in L^q(Q)$ – then we take the test function in (5.58), $v_{\varepsilon,\tau}$ as its piecewise constant approximation such that $v_{\varepsilon,\tau} \to v_\varepsilon$ strongly on $L^q(Q;\mathbb{R}^{M+1})$ and moreover $v_{\varepsilon,\tau}(t) \in L^{2q}(\Omega;\mathbb{R}^{M+1})$ for all $t \in [0,T]$ and $\|v_{\varepsilon,\tau}\|_{L^{2q}(Q;\mathbb{R}^{M+1})} \le C\tau^{\frac{-1}{2q+1}}$.

Using weak lower semi-continuity properties for the convex terms $\delta^*_S(\dot{\lambda}_{\varepsilon,\tau}) + \frac{\alpha}{q}|\dot{\lambda}_{\varepsilon,\tau}|^q$ of the left-hand side of (5.58), we get that

$$\int_0^T\!\!\int_\Omega \delta^*_S(\dot{\lambda}_\varepsilon) + \frac{\alpha}{q}|\dot{\lambda}_\varepsilon|^q \,\mathrm{d}x\,\mathrm{d}t \le \liminf_{\tau\to0} \int_0^T\!\!\int_\Omega \delta^*_S(\dot{\lambda}_{\varepsilon,\tau}) + \frac{\alpha}{q}|\dot{\lambda}_{\varepsilon,\tau}|^q \,\mathrm{d}x\,\mathrm{d}t + \int_\Omega \tau|\bar{\lambda}_{\varepsilon,\tau}(T)|^{2q} \,\mathrm{d}x.$$

As to the convergence right-hand-side of the flow rule, we use that $\Theta(\underline{w}_{\varepsilon,\tau}) \to \Theta(w)$ in $L^{q'}(Q)$ to pass to the limit in $\int_Q \Theta(\underline{w}_{\varepsilon,\tau} - \theta_{\mathrm{tr}})\vec{a}\cdot(v_{\varepsilon,\tau} - \dot{\lambda}_{\varepsilon,\tau}) \,\mathrm{d}x\,\mathrm{d}t$. Thanks to (5.41) $\tau\int_\Omega |\lambda_0|^{2q} \,\mathrm{d}x$ converges to zero. Also the term $2q\tau|\bar{\lambda}_{\varepsilon,\tau}|^{2q-2}\bar{\lambda}_{\varepsilon,\tau}v_{\varepsilon,\tau}$ can be pushed to

zero thanks to (5.48) and the blow-up for $v_{\varepsilon,\tau}$ specified above that allow us to estimate $\big|\int_Q 2q\tau|\bar\lambda_{\varepsilon,\tau}|^{2q-2}\bar\lambda_{\varepsilon,\tau}v_{\varepsilon,\tau}\big|\,\mathrm{d}x\,\mathrm{d}t \le 2q\tau\|\bar\lambda_{\varepsilon,\tau}\|^{2q-1}_{L^{(2q)}(Q;\mathbb{R}^{M+1})}\|v_{\varepsilon,\tau}\|_{L^{2q}(Q;\mathbb{R}^{M+1})} \le C\tau^{\frac{1}{4q^2+2q}}$.

For the term $\mathcal{Q}'_\varkappa\big(\bar\lambda_{\varepsilon,\tau}-L(\nabla\bar y_{\varepsilon,\tau})\big)\cdot(v_{\varepsilon,\tau}-\dot\lambda_{\varepsilon,\tau})$, we realize that, due to the compactness of $\mathcal{Q}_\varkappa(\cdot)$, $\mathcal{Q}'_\varkappa\big(\bar\lambda_{\varepsilon,\tau}(t)-L(\nabla\bar y_{\varepsilon,\tau}(t))\big)\to\mathcal{Q}'_\varkappa\big(\lambda_\varepsilon(t)-L(\nabla y_\varepsilon(t))\big)$ strongly in $L^2(\Omega;\mathbb{R}^{M+1})$ for all $t\in[0,T]$; therefore, we get by employing the Lebesgue's dominated convergence theorem that $\mathcal{Q}'_\varkappa\big(\bar\lambda_{\varepsilon,\tau}-L(\nabla\bar y_{\varepsilon,\tau})\big)\to\mathcal{Q}'_\varkappa\big(\lambda_\varepsilon-L(\nabla y_\varepsilon)\big)$ strongly also in $L^2(Q;\mathbb{R}^{M+1})$. This immediately implies that

$$\int_Q \mathcal{Q}'_\varkappa\big(\bar\lambda_{\varepsilon,\tau}-L(\nabla\bar y_{\varepsilon,\tau})\big)\cdot(v_{\varepsilon,\tau}-\dot\lambda_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t \to \int_Q \mathcal{Q}'_\varkappa\big(\lambda_\varepsilon-L(\nabla y_\varepsilon)\big)\cdot(v_\varepsilon-\dot\lambda_\varepsilon)\,\mathrm{d}x\,\mathrm{d}t.$$

Combining all above said, yields (5.33).

Step 5: Strong convergence of $\dot\lambda_{\varepsilon,\tau}$
First, we test the discrete flow rule (cf. (5.58), *reformulated using the convexity of* $|\cdot|^q$) by $\dot\lambda_{\mathrm{S},\varepsilon,\tau}$ being a piecewise constant approximation of the function $\dot\lambda$ such that $\dot\lambda_{\mathrm{S},\varepsilon,\tau}\to\dot\lambda$ strongly in $L^q(Q;\mathbb{R}^{M+1})$ and moreover $\|\dot\lambda_{\mathrm{S},\varepsilon,\tau}\|_{L^{2q}(Q;\mathbb{R}^{M+1})}\le C\tau^{-1/(2q+1)}$. We get

$$\begin{aligned}
&\int_Q \delta_S^*(\dot\lambda_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t+\int_\Omega \tau|\bar\lambda_{\varepsilon,\tau}(T)|^{2q}\,\mathrm{d}x \le \int_\Omega \tau|\lambda_{0,\varepsilon,\tau}|^{2q}\,\mathrm{d}x+\int_Q 2q\tau|\bar\lambda_{\varepsilon,\tau}|^{2q-2}\bar\lambda_{\varepsilon,\tau}\cdot\dot\lambda_{\mathrm{S},\varepsilon,\tau}\,\mathrm{d}x\,\mathrm{d}t\\
&+\int_Q \mathcal{Q}'_\varkappa\big(\bar\lambda_{\varepsilon,\tau}-L(\nabla\bar y_{\varepsilon,\tau})\big)\cdot(\dot\lambda_{\mathrm{S},\varepsilon,\tau}-\dot\lambda_{\varepsilon,\tau})+\delta_S^*(\dot\lambda_{\mathrm{S},\varepsilon,\tau})+\alpha|\dot\lambda_{\varepsilon,\tau}|^{q-2}\dot\lambda_{\varepsilon,\tau}\cdot(\dot\lambda_{\mathrm{S},\varepsilon,\tau}-\dot\lambda_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t\\
&+\int_Q \big(\Theta(\underline{w}_{\varepsilon,\tau})-\theta_{\mathrm{tr}}\big)\vec a\cdot(\dot\lambda_{\mathrm{S},\varepsilon,\tau}-\dot\lambda_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t. \qquad (5.59)
\end{aligned}$$

Symmetrically, we test the continuous flow rule (5.33) *reformulated* as above by $\dot\lambda_{\varepsilon,\tau}$ to get

$$\begin{aligned}
\int_Q \delta_S^*(\dot\lambda_\varepsilon)\,\mathrm{d}x\,\mathrm{d}t &\le \int_Q \mathcal{Q}'_\varkappa(\lambda_\varepsilon-L(\nabla y_\varepsilon))\cdot(\dot\lambda_{\varepsilon,\tau}-\dot\lambda_\varepsilon)+\delta_S^*(\dot\lambda_{\varepsilon,\tau})\\
&\quad+\int_\Omega\Big(\alpha|\dot\lambda_\varepsilon|^{q-2}\dot\lambda_\varepsilon\cdot(\dot\lambda_{\varepsilon,\tau}-\dot\lambda_\varepsilon)+(\Theta(w_\varepsilon)-\theta_{\mathrm{tr}})\vec a\cdot(\dot\lambda_{\varepsilon,\tau}-\dot\lambda_\varepsilon)\Big)\,\mathrm{d}x\,\mathrm{d}t. \qquad (5.60)
\end{aligned}$$

We add (5.59) and (5.60), apply Hölder inequality and $\lim_{\tau\to0}$ to estimate

$$\begin{aligned}
&\alpha\lim_{\tau\to0}\Big(\|\dot\lambda_{\varepsilon,\tau}\|^{q-1}_{L^q(Q;\mathbb{R}^{M+1})}-\|\dot\lambda_\varepsilon\|^{q-1}_{L^q(Q;\mathbb{R}^{M+1})}\Big)\Big(\|\dot\lambda_{\varepsilon,\tau}\|_{L^q(Q;\mathbb{R}^{M+1})}-\|\dot\lambda_\varepsilon\|_{L^q(Q;\mathbb{R}^{M+1})}\Big)\\
&\quad\le\lim_{\tau\to0}\alpha\int_Q\Big(|\dot\lambda_{\varepsilon,\tau}|^{q-2}\dot\lambda_{\varepsilon,\tau}-|\dot\lambda_\varepsilon|^{q-2}\dot\lambda_\varepsilon\Big)\cdot(\dot\lambda_{\varepsilon,\tau}-\dot\lambda_\varepsilon)\,\mathrm{d}x\,\mathrm{d}t\\
&\quad\le\lim_{\tau\to0}\Bigg(\int_Q\underbrace{\alpha|\dot\lambda_{\varepsilon,\tau}|^{q-2}\dot\lambda_{\varepsilon,\tau}(\dot\lambda_{\mathrm{S},\varepsilon,\tau}-\dot\lambda_\varepsilon)+\delta_S^*(\dot\lambda_{\mathrm{S},\varepsilon,\tau})-\delta_S^*(\dot\lambda_\varepsilon)}_{\text{(I)}}\,\mathrm{d}x\,\mathrm{d}t+\int_\Omega\underbrace{\tau|\lambda_{0,\varepsilon,\tau}|^{2q}}_{\text{(II)}}\\
&\qquad+\int_Q\underbrace{(\Theta(\underline{w}_{\varepsilon,\tau})-\theta_{\mathrm{tr}})\vec a\cdot(\dot\lambda_{\mathrm{S},\varepsilon,\tau}-\dot\lambda_{\varepsilon,\tau})+(\Theta(w_\varepsilon)-\theta_{\mathrm{tr}})\vec a\cdot(\dot\lambda_{\varepsilon,\tau}-\dot\lambda_\varepsilon)}_{\text{(III)}}\,\mathrm{d}x\,\mathrm{d}t\\
&\qquad+\int_Q\underbrace{\mathcal{P}_\varkappa(\nabla y_\varepsilon,\lambda_\varepsilon)\cdot(\dot\lambda_{\varepsilon,\tau}-\dot\lambda_\varepsilon)}_{\text{(IV)}}+\underbrace{\mathcal{P}_\varkappa(\nabla\bar y_{\varepsilon,\tau},\lambda_{\varepsilon,\tau})\cdot(\dot\lambda_{\mathrm{S},\varepsilon,\tau}-\dot\lambda_{\varepsilon,\tau})}_{\text{(V)}}\,\mathrm{d}x\,\mathrm{d}t\\
&\qquad+\int_Q\underbrace{2q\tau|\bar\lambda_{\varepsilon,\tau}|^{2q-2}\bar\lambda_{\varepsilon,\tau}\dot\lambda_{\mathrm{S},\varepsilon,\tau}}_{\text{(VI)}}\,\mathrm{d}x\,\mathrm{d}t\Bigg)\le0.
\end{aligned}$$

When passing to the limit on the right-hand-side, we use that $\dot\lambda_{\mathrm{S},\varepsilon,\tau}\to\dot\lambda_\varepsilon$ in $L^q(Q;\mathbb{R}^{M+1})$ to pass to 0 in Term (I); Term (II) converges also to 0 by exploiting (5.41). When turning to Term (III), we apply (5.55) to find this term approaching again 0; for Term (IV) we apply to the same end (5.54) combined with the fact that $\dot\lambda_{\mathrm{S},\varepsilon,\tau}\to\dot\lambda_\varepsilon$ in $L^q(Q;\mathbb{R}^{d+1})$. Term (V) can be pushed to 0 similarly as when passing to the limit in the flow rule using the available blow-up conditions. Finally, for Term (VI), we use that of $\Theta(\underline{w}_{\varepsilon,\tau})\to\Theta(w_\varepsilon)$ in $L^{q'}(Q)$ to see its limit being 0.

Using all above said, we arrive at the conclusion that $\|\dot\lambda_\tau\|_{L^q(Q;\mathbb{R}^{M+1})}\to\|\dot\lambda\|_{L^q(Q;\mathbb{R}^{M+1})}$. Hence, by the local convexity of $L^q(Q;\mathbb{R}^{M+1})$, the already proved weak convergence $\dot\lambda_\tau\to\dot\lambda$ in $L^q(Q;\mathbb{R}^{M+1})$ turns to be strong.

Step 6: Mechanic energy equality
In this step we shall establish (5.31). For this, we first establish the discrete equivalent of

$$\begin{aligned}\mathfrak{G}_\varepsilon(T,y_\varepsilon(T),\lambda_\varepsilon(T))+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T])\le\mathfrak{G}_\varepsilon(0,y_{0,\varepsilon},\lambda_{0,\varepsilon})\\+\int_0^T\langle[\mathfrak{G}_\varepsilon]'_\lambda(t,y_\varepsilon(t),\lambda_\varepsilon(t)),\dot\lambda_\varepsilon\rangle+[\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon(t),\lambda_\varepsilon(t))\,\mathrm{d}t.\end{aligned}\tag{5.61}$$

To this goal, we test, for some $l\in 1\dots N$, the minimization principle (5.40a) by $(\bar y_{\varepsilon,\tau}(t_l),\bar\lambda_{\varepsilon,\tau}(t_j))$ which leads (in terms of the mechanic part of the Gibbs free energy) to

$$\mathfrak{G}_\varepsilon(t_l,\bar y_{\varepsilon,\tau}(t_l),\bar\lambda_{\varepsilon,\tau}(t_l))+\int_\Omega\varepsilon|\nabla\bar y_{\varepsilon,\tau}(t_l)-\nabla\bar y_{\varepsilon,\tau}(t_{l-1})|\,\mathrm{d}x\le\mathfrak{G}_\varepsilon(t_l,\bar y_{\varepsilon,\tau}(t_{l-1}),\bar\lambda_{\varepsilon,\tau}(t_l)).\tag{5.62}$$

Rewriting the right-hand side, using the convexity of $\mathfrak{G}$ in λ, by means of the discrete chain rule [16] leads to

$$\begin{aligned}\mathfrak{G}_\varepsilon(t_l,\bar y_{\varepsilon,\tau}(t_{l-1}),\bar\lambda_{\varepsilon,\tau}(t_l))\le\mathfrak{G}_\varepsilon(t_{l-1},\bar y_{\varepsilon,\tau}(t_{l-1}),\bar\lambda_{\varepsilon,\tau}(t_{l-1}))\\+\int_{t_{l-1}}^{t_l}[\mathfrak{G}_\varepsilon]'_t(t,\bar y_{\varepsilon,\tau}(t_{l-1}))+\int_\Omega\mathcal{Q}'_\varkappa\big(\bar\lambda_{\varepsilon,\tau}(t)-L(\nabla\bar y_{\varepsilon,\tau}(t_{l-1}))\big)\cdot\dot\lambda_{\varepsilon,\tau}(t)\,\mathrm{d}x\,\mathrm{d}t,\end{aligned}$$

and summing this expression from $1\dots N$ gives

$$\begin{aligned}\mathfrak{G}_\varepsilon(T,\bar y_{\varepsilon,\tau}(T),\bar\lambda_{\varepsilon,\tau}(T))+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla\bar y_{\varepsilon,\tau};\Omega\times[0,T])\le\mathfrak{G}_\varepsilon(0,\bar y_{\varepsilon,\tau}(0),\bar\lambda_{\varepsilon,\tau}(0))\\+\int_0^T\Big([\mathfrak{G}_\varepsilon]'_t(t,\bar y_{\varepsilon,\tau}(t-\tau))+\int_\Omega\mathcal{Q}'_\varkappa\big(\bar\lambda_{\varepsilon,\tau}(t)-L(\nabla\bar y_{\varepsilon,\tau}(t-\tau))\big)\cdot\dot\lambda_{\varepsilon,\tau}(t)\,\mathrm{d}x\Big)\,\mathrm{d}t.\end{aligned}\tag{5.63}$$

We shall now apply $\liminf_{\tau\to0}$ to the left hand side of (5.63) which leads to

$$\begin{aligned}\mathfrak{G}_\varepsilon(T,y_\varepsilon(T),\lambda_\varepsilon(t))+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T])\\\le\liminf_{\tau\to0}\mathfrak{G}_\varepsilon(T,\bar y_{\varepsilon,\tau}(T),\bar\lambda_{\varepsilon,\tau}(T))+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla\bar y_{\varepsilon,\tau};\Omega\times[0,T])\\\le\limsup_{\tau\to0}\mathfrak{G}_\varepsilon(T,\bar y_{\varepsilon,\tau}(T),\bar\lambda_{\varepsilon,\tau}(T))+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla\bar y_{\varepsilon,\tau};\Omega\times[0,T]),\end{aligned}\tag{5.64}$$

due to the lower semi-continuity of the mechanic part of the Gibbs free energy and the

[16] See also (Benešová, Kružík and Roubíček, 2012; Roubíček, 2010) for details.

variation. Applying now $\limsup_{\tau\to\infty}$ also the right-hand side of (5.63) gives

$$\begin{aligned}
&\limsup_{\tau\to 0}\,\mathfrak{G}_\varepsilon(T,\bar y_{\varepsilon,\tau}(T),\bar\lambda_{\varepsilon,\tau}(T))+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla\bar y_{\varepsilon,\tau};\Omega\times[0,T]) \qquad (5.65)\\
&\quad\le \limsup_{\tau\to 0}\,\Big(\mathfrak{G}_\varepsilon(0,\bar y_{\varepsilon,\tau}(0),\bar\lambda_{\varepsilon,\tau}(0))\\
&\qquad+\int_0^T\Big([\mathfrak{G}_\varepsilon]'_t(t,\bar y_{\varepsilon,\tau}(t-\tau))+\int_\Omega\mathcal{Q}'_\varkappa\big(\bar\lambda_{\varepsilon,\tau}(t)-L(\nabla\bar y_{\varepsilon,\tau}(t-\tau))\big)\cdot\dot\lambda_{\varepsilon,\tau}(t)\,\mathrm{d}x\Big)\,\mathrm{d}t\Big)\\
&\quad=\mathfrak{G}_\varepsilon(0,y_\varepsilon(0),\lambda_\varepsilon(0))\\
&\qquad+\int_0^T\Big([\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon(t))+\int_\Omega\mathcal{Q}'_\varkappa\big(\lambda_\varepsilon(t)-L(y_\varepsilon(t))\big)\cdot\dot\lambda_\varepsilon(t)\,\mathrm{d}x\Big)\,\mathrm{d}t, \qquad (5.66)
\end{aligned}$$

where we used that $\int_0^T\langle[\mathfrak{G}_\varepsilon]'_\lambda(t,y_\varepsilon(t),\lambda_\varepsilon(t)),\dot\lambda_\varepsilon\rangle=\int_Q\mathcal{Q}'_\varkappa\big(\bar\lambda_\varepsilon-L(\nabla\bar y_\varepsilon)\big)\cdot(\dot\lambda_\varepsilon)\,\mathrm{d}x\,\mathrm{d}t$ converges $\int_0^T\langle[\mathfrak{G}_\varepsilon]'_\lambda(t,y_\varepsilon(t-\tau),\lambda_\varepsilon(t)),\dot\lambda_\varepsilon\rangle=\int_Q\mathcal{Q}'_\varkappa\big(\lambda_\varepsilon-L(\nabla y_\varepsilon)\big)\cdot\dot\lambda_\varepsilon\,\mathrm{d}x\,\mathrm{d}t$, as already explained in *Step 4*. Moreover, due to estimate (5.46) (line 3), $\bar y_{\varepsilon,\tau}(t-\tau)\rightharpoonup y_\varepsilon(t)$ in $L^p([0,T];W^{1,p}(\Omega;\mathbb{R}^d))$ and hence $\int_0^T[\mathfrak{G}_\varepsilon]'_t(t,\bar y_{\varepsilon,\tau}(t-\tau))\,\mathrm{d}t\to\int_0^T[\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon(t))\,\mathrm{d}t$.

Combining (5.64) and (5.66) readily gives (5.61); let us, therefore, concentrate on the opposite inequality:

$$\begin{aligned}
&\mathfrak{G}_\varepsilon(T,y_\varepsilon(T),\lambda_\varepsilon(T))+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T])\ge\mathfrak{G}_\varepsilon(0,y^{0,\varepsilon},\lambda^{0,\varepsilon})\\
&\qquad+\int_0^T[\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon(t),\lambda_\varepsilon(t))+\int_\Omega\mathcal{Q}'_\varkappa\big(\lambda_\varepsilon-L(\nabla y_\varepsilon)\big)\cdot\dot\lambda_\varepsilon\,\mathrm{d}x\,\mathrm{d}t. \qquad (5.67)
\end{aligned}$$

As was realized in e.g. (Francfort and Mielke, 2006; Kružík et al., 2005; Roubíček, 2010), (5.67) is actually a consequence of (5.30). To see this, we introduce an arbitrary partition $0=t_0^\beta<t_1^\beta<\ldots<t_{k(\beta)}^\beta=T$, with $\max_{i=1,\ldots,k}(t_i^\beta-t_{i-1}^\beta)\le\beta$, of the interval $[0,T]$. Then, from (5.30), we have

$$\begin{aligned}
\mathfrak{G}_\varepsilon(t_{i-1}^\beta,y(t_{i-1}^\beta),\lambda(t_{i-1}^\beta))&\le\mathfrak{G}_\varepsilon(t_{i-1}^\beta,y(t_i^\beta),\lambda(t_{i-1}^\beta))+\int_\Omega\varepsilon|\nabla y(t_i^\beta)-y(t_{i-1}^\beta)|\,\mathrm{d}x\\
&=\mathfrak{G}_\varepsilon(t_i^\beta,y(t_i^\beta),\lambda(t_i^\beta))+\int_\Omega\varepsilon|\nabla y(t_i^\beta)-y(t_{i-1}^\beta)|\,\mathrm{d}x\\
&\quad-\int_{t_{i-1}^\beta}^{t_i^\beta}[\mathfrak{G}_\varepsilon]'_t(t,y(t_i^\beta))+\langle[\mathfrak{G}_\varepsilon]'_\lambda(y(t_i^\beta),\lambda(t)),\dot\lambda(t)\rangle\,\mathrm{d}t.
\end{aligned}$$

Summing this expression for $i=1,...,k(\beta)$ leads to

$$\begin{aligned}
&\mathfrak{G}_\varepsilon(T,y_\varepsilon(T),\lambda_\varepsilon(T))+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T])-\mathfrak{G}(0,y_\varepsilon(0),\lambda_\varepsilon(0))\\
&\quad\ge\mathfrak{G}_\varepsilon(T,y_\varepsilon(T),\lambda_\varepsilon(T))+\sum_{i=1}^{k(\beta)}\int_\Omega\varepsilon|\nabla y_\varepsilon(t_i^\beta)-y_\varepsilon(t_{i-1}^\beta)|\,\mathrm{d}x-\mathfrak{G}(0,y_\varepsilon(0),\lambda_\varepsilon(0))\\
&\qquad\ge\sum_{i=1}^{k(\beta)}\int_{t_{i-1}^\beta}^{t_i^\beta}\mathfrak{G}'_t(t,y_\varepsilon(t_i^\beta))+\langle[\mathfrak{G}_\varepsilon]'_\lambda(y_\varepsilon(t_i^\beta),\lambda_\varepsilon(t)),\dot\lambda_\varepsilon(t)\rangle\,\mathrm{d}t\\
&=\sum_{i=1}^{k}\int_{t_{i-1}^\beta}^{t_i^\beta}\Big(\int_\Omega\underbrace{\mathcal{Q}'_\varkappa(\lambda_\varepsilon(t)-\lambda(t_i^\beta))\cdot\dot\lambda_\varepsilon(t)}_{=S_1}+\underbrace{\mathcal{Q}'_\varkappa(\lambda_\varepsilon(t_i^\beta)-L(\nabla y_\varepsilon(t_i^\beta)))\cdot\dot\lambda_\varepsilon(t_i^\beta)}_{=S_2}\,\mathrm{d}x\\
&\quad+\int_\Omega\underbrace{\mathcal{Q}'_\varkappa(\lambda_\varepsilon(t_i^\beta)-L(\nabla y_\varepsilon(t_i^\beta)))\cdot(\dot\lambda_\varepsilon(t)-\dot\lambda_\varepsilon(t_i^\beta))}_{=S_3}\,\mathrm{d}x+\underbrace{\mathfrak{G}'_t(t,y_\varepsilon(t_i^\beta))}_{=S_4}\Big)\,\mathrm{d}t. \qquad (5.68)
\end{aligned}$$

To pass to the limit $\beta \to 0$ on the right-hand side, we exploit[17] (Dal Maso et al., 2005, Lemma 4.12) that for any Bochner integrable $h : [0,T] \mapsto X$, where X is a Banach space, assures the existence of sequence of partitions $0 = t_0^\beta < t_1^\beta < \ldots < t_{k(\beta)}^\beta = T$ with $\max_{i=1,\ldots,k(\beta)}(t_i^\beta - t_{i-1}^\beta) \leq \beta$ such that

$$\lim_{\beta\to 0} \sum_{i=1}^{k(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} \|h(t) - h(t_i^\beta)\|_X \,\mathrm{d}t = 0,$$

or, in other words, the piecewise constant interpolant of h denoted h_β such that $h_\beta(t) = h(t_i^\beta)$ on $[t_{i-1}^\beta, t_i^\beta)$ converges strongly to h in $L^1([0,T];X)$.

Further, if $h \in L^p(Q;\mathbb{R}^s)$ for some $p > 1$, the above mentioned lemma implies that also $h_\beta \rightharpoonup h$ weakly $L^p(Q;\mathbb{R}^s)$, cf. (Benešová and Roubíček, 2012; Roubíček, 2011).

Note that (Dal Maso et al., 2005, Lemma 4.12) and its corollary hold with the same sequence of partitions for finitely many functions, since we may always choose h in the form of a vector. Hence, we can assume that our sequence of partitions $0 \leq t_1^\beta < \ldots < t_{k(\beta)}^\beta = T$ is chosen in such a way that simultaneously[18]

$$\lambda_\beta \rightharpoonup \lambda \qquad \text{weakly in } L^q(Q), \tag{5.69a}$$
$$[y_\varepsilon]_\beta \rightharpoonup y_\varepsilon \qquad \text{weakly in } L^p([0,T],W^{1,p}(\Omega;\mathbb{R}^d)), \tag{5.69b}$$
$$[\dot\lambda_\varepsilon]_\beta \to \dot\lambda_\varepsilon \qquad \text{strongly in } L^1([0,T];L^q(\Omega)), \text{ and} \tag{5.69c}$$
$$\big[\textstyle\int_\Omega \mathcal{Q}'_\varkappa(\lambda_\varepsilon - L(\nabla y_\varepsilon))\dot\lambda_\varepsilon \,\mathrm{d}x\big]_\beta \to \int_\Omega \mathcal{Q}'_\varkappa(\lambda_\varepsilon - L(\nabla y_\varepsilon))\dot\lambda_\varepsilon \,\mathrm{d}x$$
$$\text{strongly in } L^1([0,T]). \tag{5.69d}$$

Exploiting (5.69b) allows us to rewrite and converge:

$$\sum_{i=1}^{k(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} S_4 \,\mathrm{d}t = \int_0^T \left(\int_\Omega \dot f \cdot [y_\varepsilon]_\beta \,\mathrm{d}x + \int_\Gamma \dot g \cdot [y_\varepsilon]_\beta \,\mathrm{d}S \right) \mathrm{d}t \to \int_0^T \mathfrak{G}'_t(t, y_\varepsilon(t)) \,\mathrm{d}t. \tag{5.70}$$

For the term S_2 we have that

$$\sum_{i=1}^{k(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} S_2 \,\mathrm{d}t = \int_0^T \big[\textstyle\int_\Omega \mathcal{Q}'_\varkappa(\lambda_\varepsilon - L(\nabla y_\varepsilon))\dot\lambda_\varepsilon \,\mathrm{d}x\big]_\beta \,\mathrm{d}t \to \int_Q \mathcal{Q}'_\varkappa(\lambda_\varepsilon - L(\nabla y_\varepsilon))\dot\lambda_\varepsilon \,\mathrm{d}x\,\mathrm{d}t \tag{5.71}$$

just by (5.69d). Owing to (5.69a), it holds

$$\sum_{i=1}^{k(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} S_1 \,\mathrm{d}t \to 0. \tag{5.72}$$

Eventually, for the term S_3 we may rewrite

$$\Big| \sum_{i=1}^{k(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} \int_\Omega \mathcal{Q}'_\varkappa\big(\lambda_\varepsilon(t_i^\beta) - L(\nabla y_\varepsilon(t_i^\beta))\big) \cdot \big(\dot\lambda_\varepsilon(t) - \dot\lambda_\varepsilon(t_i^\beta)\big) \,\mathrm{d}t \Big|$$
$$\leq \sum_{i=1}^{k(\beta)} C \sup_{t\in[0,T]} \|\mathcal{Q}'_\varkappa(\lambda_\varepsilon(t) - L(\nabla y_\varepsilon(t)))\|_{L^2(\Omega)} \int_{t_{i-1}^\beta}^{t_i^\beta} \|[\dot\lambda_\varepsilon]_\beta - \dot\lambda_\varepsilon\|_{L^q(\Omega)} \,\mathrm{d}t \to 0, \tag{5.73}$$

[17] The procedure here is taken from (Benešová and Roubíček, 2012) where it was inspired by (Roubíček, 2011).

[18] In fact, one could even assume that $y_{\varepsilon,\beta} \to y_\varepsilon$ *strongly* in (5.69c), but only in $L^1([0,T],W^{1,p}(\Omega;\mathbb{R}^d))$

as $\sup_{t\in[0,T]}\|\lambda_\varepsilon(t)-L(\nabla y_\varepsilon(t))\|_{L^2(\Omega)}$ and, in turn, $\sup_{t\in[0,T]}\|\mathcal{Q}'_\varkappa(\lambda_\varepsilon(t)-L(\nabla y_\varepsilon(t)))\|_{L^2(\Omega)}$ are bounded independently of β and because of the strong convergence of $[\dot\lambda_\varepsilon]_\beta$ highlighted above. Merging (5.70)–(5.73) with (5.68) yields the desired inequality (5.67).

Finally, using (5.67) in (5.64) and (5.66) yields after reformulating

$$\begin{aligned}
&\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T]) \le \liminf_{\tau\to0}\varepsilon\mathrm{Var}_{|\cdot|}(\nabla\bar y_{\varepsilon,\tau};\Omega\times[0,T]) \le \limsup_{\tau\to0}\varepsilon\mathrm{Var}_{|\cdot|}(\nabla\bar y_{\varepsilon,\tau};\Omega\times[0,T])\\
&\quad\le \limsup_{\tau\to0}\Big(\mathfrak{G}_\varepsilon(0,\bar y_{\varepsilon,\tau}(0),\bar\lambda_{\varepsilon,\tau}(0)) - \mathfrak{G}_\varepsilon(T,\bar y_{\varepsilon,\tau}(T),\bar\lambda_{\varepsilon,\tau}(T))\\
&\qquad+\int_0^T\Big([\mathfrak{G}_\varepsilon]'_t(t,\bar y_{\varepsilon,\tau}(t-\tau))+\int_\Omega\mathcal{Q}'_\varkappa\big(\bar\lambda_{\varepsilon,\tau}(t)-L(\nabla\bar y_{\varepsilon,\tau}(t-\tau))\big)\cdot\dot\lambda_{\varepsilon,\tau}(t)\,\mathrm{d}x\Big)\,\mathrm{d}t\Big)\\
&\quad=\Big(\mathfrak{G}_\varepsilon(0,y_\varepsilon(0),\lambda_\varepsilon(0)) - \mathfrak{G}_\varepsilon(T,y_\varepsilon(T),\lambda_\varepsilon(T))\\
&\qquad+\int_0^T\Big([\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon(t))+\int_\Omega\mathcal{Q}'_\varkappa\big(\lambda_\varepsilon(t)-L(\nabla y_\varepsilon(t))\big)\cdot\dot\lambda_\varepsilon(t)\,\mathrm{d}x\Big)\,\mathrm{d}t\Big)\\
&\le\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T]),
\end{aligned}\tag{5.74}$$

i.e., since all inequalities are actually equalities,

$$\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T]) = \lim_{\tau\to0}\varepsilon\mathrm{Var}_{|\cdot|}(\nabla\bar y_{\varepsilon,\tau};\Omega\times[0,T]).\tag{5.75}$$

Step 7: Convergence of the enthalpy equation.
Performing discrete by parts integration in (5.40b) summed from 1 to N yields

$$\begin{aligned}
-\int_0^T\Big(\int_\Omega\bar w_{\varepsilon,\tau}\dot{\bar\varphi}+\mathcal{K}(\bar\lambda_{\varepsilon,\tau},\bar w_{\varepsilon,\tau})\nabla\bar w_{\varepsilon,\tau}\cdot\nabla\bar\varphi\,\mathrm{d}x+\int_\Gamma\bar b_{\varepsilon,\tau}\Theta(\bar w_{\varepsilon,\tau})\bar\varphi\,\mathrm{d}S\Big)\,\mathrm{d}t = \int_\Omega w^0_{\varepsilon,\tau}\bar\varphi(0)\,\mathrm{d}x\\
+\int_0^{t_k}\Big(\int_\Omega\big(\varrho_q(\dot\lambda_{\varepsilon,\tau})+\varepsilon|\dot y_{\varepsilon,\tau}|\big)\bar\varphi+\Theta(\bar w_{\varepsilon,\tau})\vec a\cdot\dot\lambda_{\varepsilon,\tau}\bar\varphi\,\mathrm{d}x+\int_\Gamma\bar b_\tau\bar\theta_{\mathrm{ext},\tau}\bar\varphi\,\mathrm{d}S\Big)\,\mathrm{d}t,
\end{aligned}\tag{5.76}$$

for all $\bar\varphi$ piecewise constant on the intervals $(t_{j-1},t_j]$ such that, for any j, $\bar\varphi(t_j,\cdot)\in W^{1,2}(\Omega)$, $\bar\varphi(T)=0$ and φ piecewise linear on the intervals $(t_{j-1},t_j]$, such that $\bar\varphi(t_j,\cdot)=\varphi(t_j,\cdot)$. Note that by such test functions we may approximate (strongly in the norm of $L^r(Q)$, $r\in[1,\infty]$) any $\tilde\varphi\in C^1(\bar Q)$.

To pass to the limit $\tau\to0$ in this equation, we make use of (5.56) to handle the term $\bar w_{\varepsilon,\tau}\dot{\bar\varphi}$; furthermore, we use that $\bar\lambda_{\varepsilon,\tau}\to\lambda_\varepsilon$ strongly in $L^q(Q;\mathbb{R}^{M+1})$ (owing to *Step 5*), which together with assumption (A5), gives $\mathcal{K}(\bar\lambda_{\varepsilon,\tau},\bar w_{\varepsilon,\tau})\to\mathcal{K}(\lambda_\varepsilon,w_\varepsilon)$ strongly in any Lebesgue space, except for $L^\infty(Q;\mathbb{R}^{d\times d})$.

Next, by the Aubin-Lions theorem and by interpolation (see (Roubíček, 2005)), we get that $\bar w_{\varepsilon,\tau}\to w_\varepsilon$ strongly in $L^{(d+2)/(d+1)-\delta}([0,T];W^{1-\delta,(d+2)/(d+1)-\delta}(\Omega))$ for any $\delta>0$ small, so that the traces converge strongly in $L^{(d+2)/(d+1)-\delta}([0,T];L^{(d^2+d-2)/(d^2-2)-\delta}(\Gamma))$. Combining that with assumption (A6) and (5.42) allows us to handle the left-hand-side boundary term.

For the right-hand-side we exploit the strong convergence $\dot\lambda_{\varepsilon,\tau}\to\dot\lambda_\varepsilon$ in $L^q(Q;\mathbb{R}^{M+1})$ to take the limit in the terms expressing dissipated heat in $\dot\lambda$. To establish the limit of $\varepsilon|\dot y_{\varepsilon,\tau}|\bar\varphi$, we exploit (5.75) and follow the procedure of (Roubíček, 2010). For the term $\Theta(\bar w_{\varepsilon,\tau})\vec a\cdot\dot\lambda_{\varepsilon,\tau}\bar\varphi$, we employ that $\Theta(\bar w_{\varepsilon,\tau})\to\Theta(w)$ in $L^{q'}(Q)$; finally, for the right-hand-side boundary term the weak convergence of $\bar b_\tau\bar\theta_{\mathrm{ext},\tau}\to b\theta_{\mathrm{ext}}$ in $L^1(Q)$ (see (5.42)) is available, which allows us to pass to the limit in this term. □

Remark 5.11 (On mathematical importance of the "pinning" term $\varepsilon|\nabla\dot y_\varepsilon|$ in (5.27)).
Let us, at this point, shortly point out the philosophy of the term $\varepsilon|\nabla\dot y_\varepsilon|$ from (5.27) –

the main purpose for including it is to get more information on the behavior "in-time" of the deformation.

Indeed the term $\varepsilon|\nabla\dot{y}_\varepsilon|$ from (5.27) was exploited already in the a-priori estimates in Lemma 5.10 yielding the third estimate in (5.46). This was subsequently exploited in *Step 3* of the above proof to get (5.52); that was again essential in *Step 4* in order to pass to the limit in the flow-rule, in particular in the term $\int_0^T\int_\Omega \mathcal{P}_\varkappa(\nabla y_{\varepsilon,\tau},\lambda_{\varepsilon,\tau})\cdot(v-\dot\lambda_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t$.

Without the added dissipation term $\varepsilon|\nabla\dot{y}_\varepsilon|$, we could only establish that for any $t\in[0,T]$ there exists a subsequence τ_t, *depending on* t, such that $\nabla y_{\varepsilon,\tau_t}(t)\to\nabla y_\varepsilon(t)$ strongly in $L^2(\Omega;\mathbb{R}^{d\times d})$. This, however, is not sufficient to pass to the limit in the in the discrete flow rule (5.58), namely the limit of the aforementioned term $\int_0^T\int_\Omega \mathcal{P}_\varkappa(\nabla y_{\varepsilon,\tau},\lambda_{\varepsilon,\tau})\cdot(v-\dot\lambda_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t$, stemming from the penalty, cannot be evaluated.

For completeness, we need to prove the a-priori estimates from Lemma 5.10; the procedure taken here follows in large parts (Benešová, Kružík and Roubíček, 2012) where also heuristics on the proof were given – the ideas in (Benešová, Kružík and Roubíček, 2012) were inspired by (Roubíček, 2010) exploiting a technique developed by Boccardo and Gallouët (Boccardo et al., 1997; Boccardo and Galloët, 1989). Recall also that in the proof we will use C as a generic constant independent of τ, ε.

Proof Lemma 5.10. For the sake of clarity, let us divide the proof into several steps.

Step 1: Using (5.63) and (5.58)
Let us estimate the left-hand side of (a slight modification of) (5.63)[19]

$$\begin{aligned}
&\int_\Omega C|\nabla\bar y_{\varepsilon,\tau}(t_k)|^p+\frac{\varepsilon}{2}|\nabla^2\bar y_{\varepsilon,\tau}(t_k)|^2\,\mathrm{d}x+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla\bar y_{\varepsilon,\tau};\Omega\times[0,t_k])-C\\
&\quad\le \mathfrak{G}_\varepsilon(t_k,\bar y_{\varepsilon,\tau}(t_k),\bar\lambda_{\varepsilon,\tau}(t_k))+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla\bar y_{\varepsilon,\tau},\Omega\times[0,t_k])\\
&\quad\le \int_0^{t_k}\Big([\mathfrak{G}_\varepsilon]'_t(t,\bar y_{\varepsilon,\tau}(t-\tau))+\int_\Omega \mathcal{Q}'_\varkappa\big(\bar\lambda_{\varepsilon,\tau}-L(\nabla\bar y_{\varepsilon,\tau}(t-\tau))\big)\cdot\dot\lambda_{\varepsilon,\tau}\Big)\,\mathrm{d}x\,\mathrm{d}t+C\\
&\quad\le \int_0^{t_k}\int_\Omega C|\nabla\bar y_{\delta,\tau}|^p+\varkappa\mathfrak{Q}\bar\lambda_{\varepsilon,\tau}\mathfrak{Q}\dot\lambda_{\varepsilon,\tau}-|\mathcal{Q}'_\varkappa\big(L(\nabla\bar y_{\varepsilon,\tau}(t-\tau))\big)|\,|\dot\lambda_{\varepsilon,\tau}|\,\mathrm{d}x\,\mathrm{d}t+C,\\
&\quad\le \int_0^{t_k}\int_\Omega C|\nabla\bar y_{\delta,\tau}|^p+\varkappa\mathfrak{Q}\bar\lambda_{\varepsilon,\tau}\mathfrak{Q}\dot\lambda_{\varepsilon,\tau}+\frac{\alpha}{3q}|\dot\lambda_{\varepsilon,\tau}|\,\mathrm{d}x\,\mathrm{d}t+C;
\end{aligned}\tag{5.77}$$

where we exploited the Hölder's and Young's inequality; for the term $|\mathcal{Q}'_\varkappa\big(L(\nabla\bar y_{\varepsilon,\tau}(t-\tau))\big)|$ we used (A3) and (A2) was exploited in $[\mathfrak{G}_\varepsilon]'_t(t,\bar y_{\delta,\tau}(t-\tau))$.[20]

[19] Obtained by exploiting (5.62) from $1\dots k$ instead of $1\dots N$ (as in the case of (5.63)) to get

$$\begin{aligned}
\mathfrak{G}_\varepsilon(t_k,\bar y_{\varepsilon,\tau}(t_k),\bar\lambda_{\varepsilon,\tau}(t_k))+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla\bar y_{\varepsilon,\tau};\Omega\times[0,t_k])&\le \mathfrak{G}_\varepsilon(0,\bar y_{\varepsilon,\tau}(0),\bar\lambda_{\varepsilon,\tau}(0))\\
&+\int_0^{t_k}\Big([\mathfrak{G}_\varepsilon]'_t(t,\bar y_{\varepsilon,\tau}(t-\tau))+\int_\Omega \mathcal{Q}'_\varkappa\big(\bar\lambda_{\varepsilon,\tau}(t)-L(\nabla\bar y_{\varepsilon,\tau}(t-\tau))\big)\cdot\dot\lambda_{\varepsilon,\tau}(t)\,\mathrm{d}x\Big)\,\mathrm{d}t.
\end{aligned}$$

[20] Note that the term $[\mathfrak{G}_\varepsilon]'_t(t,\bar y_{\varepsilon,\tau}(t-\tau))=\int_\Omega \dot f(t)\bar y_{\varepsilon,\tau}(t-\tau)\,\mathrm{d}x+\int_{\Gamma_\mathrm{N}}\dot g(t)\bar y_{\varepsilon,\tau}(t-\tau)\,\mathrm{d}S$ may be estimated, using (A3) combined with the Hölder's and Young's inequality, as follows (for simplicity we demonstrate the procedure only for $\int_\Omega \dot f(t)\bar y_{\varepsilon,\tau}(t-\tau)\,\mathrm{d}x$, for $\int_{\Gamma_\mathrm{N}}\dot g(t)\bar y_{\varepsilon,\tau}(t-\tau)\,\mathrm{d}S$ we would proceed analogously):

Next, using $v_{\varepsilon,\tau} = 0$ in (a slight modification of) (5.58) [21] leads, when recalling definition (5.2), to

$$\begin{aligned}
&\int_0^{t_k}\int_\Omega \delta_S^*(\dot{\bar\lambda}_{\varepsilon,\tau}) + \frac{\alpha}{q}|\dot{\bar\lambda}_{\varepsilon,\tau}|^q \,\mathrm{d}x\,\mathrm{d}t + \frac{\varkappa}{2}\|\mathfrak{Q}\bar\lambda_{\varepsilon,\tau}(t_k)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})} + \int_\Omega \tau|\bar\lambda_{\varepsilon,\tau}(t_k)|^{2q}\,\mathrm{d}x\\
&\quad\le \int_0^{t_k}\int_\Omega \Big(\varkappa|\mathfrak{Q}L(\nabla\bar y_{\varepsilon,\tau}(t-\tau))|\,|\mathfrak{Q}\dot{\bar\lambda}_{\varepsilon,\tau}| + |\Theta(\underline{w}_{\varepsilon,\tau}) - \theta_{\mathrm{tr}}|\,|\vec a|\,|\dot{\bar\lambda}_{\varepsilon,\tau}|\,\mathrm{d}x\Big)\,\mathrm{d}t\\
&\qquad\qquad + \|\mathfrak{Q}\bar\lambda_{\varepsilon,\tau}(0)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})} + \int_\Omega \tau|\bar\lambda_{\varepsilon,\tau}(0)|^{2q}\,\mathrm{d}x\\
&\quad\le \int_0^{t_k}\int_\Omega \Big(\frac{\alpha}{6qc_{\mathrm{em}}}\|\mathfrak{Q}\dot{\bar\lambda}_{\varepsilon,\tau}\|^q + C|\Theta(\underline{w}_{\varepsilon,\tau}) - \theta_{\mathrm{tr}}|^{q'} + \frac{\alpha}{6q}|\dot{\bar\lambda}_{\varepsilon,\tau}|^q\,\mathrm{d}x\Big)\,\mathrm{d}t + C\\
&\quad\le \int_0^{t_k}\int_\Omega C|\underline{w}_{\varepsilon,\tau}| + \frac{\alpha}{3q}|\dot{\bar\lambda}_{\varepsilon,\tau}|^q\,\mathrm{d}x\,\mathrm{d}t + \tau\|\lambda_{0,\tau}\|^{2q}_{L^{2q}(\Omega;\mathbb{R}^{M+1})} + C,
\end{aligned}\tag{5.78}$$

by first exploiting the *discrete chain rule*[22] and subsequently applying the Young's inequality to the terms $\varkappa|\mathfrak{Q}L(\nabla\bar y_{\varepsilon,\tau}(t-\tau))|\,|\mathfrak{Q}\dot{\bar\lambda}_{\varepsilon,\tau}|$ as well as $|\Theta(\underline{w}_{\varepsilon,\tau}) - \theta_{\mathrm{tr}}||\vec a||\dot{\bar\lambda}_{\varepsilon,\tau}|$. Further, we estimated $\varkappa|\mathfrak{Q}L(\nabla\bar y_{\varepsilon,\tau}(t-\tau))| \le C$ (due to (A3)) and, as $q \ge 2$ we may write $\int_\Omega |\mathfrak{Q}\dot{\bar\lambda}_{\varepsilon,\tau}|\,\mathrm{d}x \le c_{\mathrm{em}}\|\dot{\bar\lambda}_{\varepsilon,\tau}\|^q_{L^q(\Omega;\mathbb{R}^{M+1})}$, with some constant c_{em}. Eventually, $|\Theta(\underline{w}_{\varepsilon,\tau})|^{q'} \le C(1+|\underline{w}_{\varepsilon,\tau}|^{q'/\omega}) \le C(1+|\underline{w}_{\varepsilon,\tau}|)$ due to assumption (A4) and $q'/\omega < 1$.

Step 2: Using the enthalpy equation (5.76)

$$\begin{aligned}
\Big|\int_0^{t_k}\int_\Omega \dot f(t)\bar y_{\varepsilon,\tau}(t-\tau)\,\mathrm{d}x\Big| &\le \int_0^{t_k} \|\dot f(t)\|_{L^{p^{*\prime}}(\Omega;\mathbb{R}^d)}\|\bar y_{\varepsilon,\tau}(t-\tau)\|_{W^{1,p}(\Omega;\mathbb{R}^d)}\,\mathrm{d}t\\
&\le C\int_0^{t_k} \|\dot f(t)\|^{p'}_{L^{p^{*\prime}}(\Omega;\mathbb{R}^d)}\,\mathrm{d}t + \int_0^{t_k}\|\bar y_{\varepsilon,\tau}(t-\tau)\|^p_{W^{1,p}(\Omega;\mathbb{R}^d)}\,\mathrm{d}t\\
&= C\int_0^{t_k} \|\dot f(t)\|^{p'}_{L^{p^{*\prime}}(\Omega;\mathbb{R}^d)}\,\mathrm{d}t + \int_\tau^{t_k}\|\bar y_{\varepsilon,\tau}(t-\tau)\|^p_{W^{1,p}(\Omega;\mathbb{R}^d)}\,\mathrm{d}t + \tau\|y^0_{\varepsilon,\tau}\|^p_{W^{1,p}(\Omega;\mathbb{R}^d)}\\
&= C\int_0^{t_k} \|\dot f(t)\|^{p'}_{L^{p^{*\prime}}(\Omega;\mathbb{R}^d)}\,\mathrm{d}t + \int_0^{t_k-\tau}\|\bar y_{\varepsilon,\tau}(t)\|^p_{W^{1,p}(\Omega;\mathbb{R}^d)}\,\mathrm{d}t + \tau\|y^0_{\varepsilon,\tau}\|^p_{W^{1,p}(\Omega;\mathbb{R}^d)}\\
&\le C\int_0^{t_k} \|f(t)\|^{p'}_{L^{p^{*\prime}}(\Omega;\mathbb{R}^d)}\,\mathrm{d}t + \int_0^{t_k}\|\bar y_{\varepsilon,\tau}(t)\|^p_{W^{1,p}(\Omega;\mathbb{R}^d)}\,\mathrm{d}t + \tau\|y^0_{\varepsilon,\tau}\|^p_{W^{1,p}(\Omega;\mathbb{R}^d)}\\
&\le C\Big(1 + \int_0^{t_k}\|\bar y_{\varepsilon,\tau}(t)\|^p_{W^{1,p}(\Omega;\mathbb{R}^d)}\,\mathrm{d}t\Big) \le C\Big(1 + \int_0^{t_k}\int_\Omega |\nabla\bar y_{\varepsilon,\tau}(t)|^p\,\mathrm{d}t\Big),
\end{aligned}$$

where, in the last line, we exploited assumption (A2) on f and (5.40d) for $y^0_{\varepsilon,\tau}$.

[21] Ones again, we use sum the partial derivatives with respect to λ of the cost function in (5.40a), being equal to 0, only from 1 to k instead of N to get

$$\begin{aligned}
\int_0^{t_k}\int_\Omega \rho_q(\dot{\bar\lambda}_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t &\le \int_0^{t_k}\int_\Omega \mathcal{Q}'_\varkappa\big(\bar\lambda_{\varepsilon,\tau} - L(\nabla\bar y_{\varepsilon,\tau})\big)\cdot(v_{\varepsilon,\tau} - \dot{\bar\lambda}_{\varepsilon,\tau}) + \rho_q(v_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t\\
&\quad + \int_0^{t_k}\int_\Omega (\Theta(\underline{w}_{\varepsilon,\tau}(t)) - \theta_{\mathrm{tr}})\vec a\cdot(v_{\varepsilon,\tau} - \dot{\bar\lambda}_{\varepsilon,\tau}) + 2q\tau|\bar\lambda_{\varepsilon,\tau}|^{2q-2}\bar\lambda_{\varepsilon,\tau}(v_{\varepsilon,\tau} - \dot{\bar\lambda}_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t.
\end{aligned}$$

[22] Indeed, by the convexity and due to definition (5.2), we may rewrite

$$\begin{aligned}
\frac{\varkappa}{2}\|\mathfrak{Q}\bar\lambda_{\varepsilon,\tau}(0)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})} - \frac{\varkappa}{2}\|\mathfrak{Q}\bar\lambda_{\varepsilon,\tau}(t_k)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})}\,\mathrm{d}x &\ge -\int_0^{t_k}\int_\Omega \mathcal{Q}'_\varkappa(\dot{\bar\lambda}_{\varepsilon,\tau})\cdot\dot{\bar\lambda}_{\varepsilon,\tau}\,\mathrm{d}t\\
\int_\Omega |\bar\lambda_{\varepsilon,\tau}(0)|^{2q} - \int_\Omega |\bar\lambda_{\varepsilon,\tau}(t_k)|^{2q}\,\mathrm{d}x &\ge -2q\int_0^{t_k}\int_\Omega \dot{\bar\lambda}_{\varepsilon,\tau}\bar\lambda_{\varepsilon,\tau}|\bar\lambda_{\varepsilon,\tau}|^{2q-2}\,\mathrm{d}x\,\mathrm{d}t.
\end{aligned}$$

In this step, we test (a modification of) (5.76)[23] by 1 to get

$$\begin{aligned}\int_0^{t_k}\!\!\int_\Omega \dot{w}_{\varepsilon,\tau}\,\mathrm{d}x\,\mathrm{d}t &\le \int_0^{t_k}\Big(\int_\Omega \dot{w}_{\varepsilon,\tau}\,\mathrm{d}x+\int_\Gamma \bar{b}_{\varepsilon,\tau}\Theta(\bar{w}_{\varepsilon,\tau})\,\mathrm{d}S\Big)\,\mathrm{d}t\\ &\le \int_0^{t_k}\Big(\int_\Omega \delta_S^*(\dot{\lambda}_{\varepsilon,\tau})+\alpha|\dot{\lambda}_{\varepsilon,\tau}|^q+\varepsilon|\dot{y}_{\varepsilon,\tau}|+|\Theta(\bar{w}_{\varepsilon,\tau})||\vec{a}||\dot{\lambda}_{\varepsilon,\tau}|+\int_\Gamma|\bar{\theta}_{\mathrm{ext},\tau}|\,\mathrm{d}x\Big)\,\mathrm{d}t\\ &\le \int_0^{t_k}\!\!\int_\Omega 2\alpha|\dot{\lambda}_{\varepsilon,\tau}|^q+C|\bar{w}_{\varepsilon,\tau}|\,\mathrm{d}x\,\mathrm{d}t+\varepsilon\mathrm{Var}_{|\cdot|}(\nabla\bar{y}_{\varepsilon,\tau};\Omega\times[0,t_k])+C \qquad (5.79)\end{aligned}$$

where we estimated the term $|\Theta(\bar{w}_{\varepsilon,\tau})||\vec{a}||\dot{\lambda}_{\varepsilon,\tau}|$ similarly as in *Step 1* and inserted the identity $\varepsilon\mathrm{Var}_{|\cdot|}(\nabla\bar{y}_{\varepsilon,\tau},[0,t_k])=\int_0^{t_k}\int_\Omega\varepsilon|\dot{y}_{\varepsilon,\tau}|\,\mathrm{d}x\,\mathrm{d}t$.

Multiplying (5.79) by $1/(12q)$ and adding to (5.78) and (5.77) gives

$$\begin{aligned}&\int_0^{t_k}\!\!\int_\Omega\frac{\alpha}{6q}|\dot{\lambda}_{\varepsilon,\tau}|^q\,\mathrm{d}x\,\mathrm{d}t+\int_\Omega\tau|\bar{\lambda}_{\varepsilon,\tau}(t_k)|^{2q}+\int_\Omega C|\nabla\bar{y}_{\varepsilon,\tau}(t_k)|^p+\frac{\varepsilon}{2}|\nabla^2\bar{y}_{\varepsilon,\tau}(t_k)|^2\,\mathrm{d}x\\ &\quad+\frac{\varepsilon}{12q}\mathrm{Var}_{|\cdot|}(\nabla\bar{y}_{\varepsilon,\tau},[0,t_k])+\int_\Omega|\bar{w}_{\varepsilon,\tau}(t_k)|\,\mathrm{d}x\\ &\qquad\le C\bigg(1+\int_0^{t_k}\!\!\int_\Omega|\bar{w}_{\varepsilon,\tau}|+|\nabla\bar{y}_{\varepsilon,\tau}|^p\,\mathrm{d}x\,\mathrm{d}t\bigg), \qquad (5.80)\end{aligned}$$

i.e. we got (5.46)-(5.49) by exploiting the discrete Gronwall inequality (Roubíček, 2005).

Step 3: Estimation of $\nabla\bar{w}_\tau$

In this step we prove (5.50). To this end, let us test (5.76) by $\eta(\bar{w}_\tau)$ where $\eta(w)=1-\frac{1}{(1+w)^a}$ with $a>0$, which, due to the non-negativity of the enthalpy is a legal test. Notice that due to the discrete chain rule, relying on the convexity of $\tilde{\eta}$, we have that

$$\int_\Omega\tilde{\eta}(T)-\tilde{\eta}(0)\,\mathrm{d}x=\int_Q\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\eta}(\bar{w}_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t\le\int_Q\dot{w}_{\varepsilon,\tau}\eta(\bar{w}_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t,$$

where $\tilde{\eta}$ denotes the primitive function of η such that $\tilde{\eta}(0)=0$. Realize also that due to the fact that $\eta(w)\ge0$ also $\tilde{\eta}(T)\ge0$ and hence we may write

$$\begin{aligned}\kappa_0 a\int_Q\frac{|\nabla\bar{w}_{\varepsilon,\tau}|^2}{(1+\bar{w})^{1+a}}\,\mathrm{d}x\,\mathrm{d}t&=\kappa_0\int_Q|\nabla\bar{w}_{\varepsilon,\tau}|^2\eta'(\bar{w}_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t\\ &\le\int_Q\overline{\mathcal{K}}\nabla\bar{w}_{\varepsilon,\tau}\cdot\nabla\bar{w}_{\varepsilon,\tau}\eta'(\bar{w}_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t=\int_Q\overline{\mathcal{K}}\nabla\bar{w}_{\varepsilon,\tau}\cdot\nabla\eta(\bar{w}_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t\\ &\le\int_\Omega\tilde{\eta}(w_{\varepsilon,\tau}(T))\,\mathrm{d}x+\int_Q\overline{\mathcal{K}}\nabla\bar{w}_{\varepsilon,\tau}\cdot\nabla\eta(\bar{w}_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t+\int_\Sigma\bar{b}_{\varepsilon,\tau}\Theta(\bar{w}_{\varepsilon,\tau})\eta(\bar{w}_{\varepsilon,\tau})\,\mathrm{d}S\,\mathrm{d}t\\ &=\int_\Sigma\bar{b}_{\varepsilon,\tau}\bar{\theta}_{\mathrm{ext},\varepsilon,\tau}\eta(\bar{w}_{\varepsilon,\tau})\,\mathrm{d}S\,\mathrm{d}t+\int_\Omega\tilde{\eta}(w_0)\,\mathrm{d}x\\ &\qquad+\int_Q(\varrho_q(\dot{\lambda}_{\varepsilon,\tau})+\Theta(\bar{w}_{\varepsilon,\tau})\vec{a}\cdot\dot{\lambda}_{\varepsilon,\tau}+\epsilon|\nabla\dot{y}_{\varepsilon,\tau}|)\eta(\bar{w}_{\varepsilon,\tau})\,\mathrm{d}x\,\mathrm{d}t\\ &\le C+\|\bar{r}_{\varepsilon,\tau}\|_{L^1(Q)} \qquad (5.81)\end{aligned}$$

[23] As above, we sum (5.40b) from 1 to k instead of N to get

$$\begin{aligned}&-\int_0^{t_k}\Big(\int_\Omega\dot{w}_{\varepsilon,\tau}\dot{\varphi}+\mathcal{K}(\bar{\lambda}_{\varepsilon,\tau},\bar{w}_{\varepsilon,\tau})\nabla\bar{w}_{\varepsilon,\tau}\nabla\bar{\varphi}\,\mathrm{d}x+\int_\Gamma\bar{b}_{\varepsilon,\tau}\Theta(\bar{w}_{\varepsilon,\tau})\bar{\varphi}\,\mathrm{d}S\Big)\,\mathrm{d}t\\ &\qquad=\int_0^{t_k}\Big(\int_\Omega(\varrho_q(\dot{\lambda}_{\varepsilon,\tau})+\varepsilon|\dot{y}_{\varepsilon,\tau}|)\bar{\varphi}+\Theta(\bar{w}_{\varepsilon,\tau})\vec{a}\cdot\dot{\lambda}_{\varepsilon,\tau}\bar{\varphi}\,\mathrm{d}x+\int_\Gamma\bar{b}_\tau\bar{\theta}_{\mathrm{ext},\tau}\bar{\varphi}\,\mathrm{d}S\Big)\,\mathrm{d}t.\end{aligned}$$

with the shorthand notation $\overline{\mathcal{K}} = \mathcal{K}(\bar\lambda_{\varepsilon,\tau}, \bar w_{\varepsilon,\tau})$ and where we used the obvious bound $|\eta(\bar w_\tau)| \le 1$ and abbreviated

$$\bar r_{\varepsilon,\tau} := \varrho_q(\dot\lambda_{\varepsilon,\tau}) + \epsilon|\nabla\dot y_{\varepsilon,\tau}| + \Theta(\bar w_{\varepsilon,\tau})\vec a\cdot\dot\lambda_{\varepsilon,\tau}.$$

Note that $\bar r_{\varepsilon,\tau}$ is bounded due to (5.46)-(5.49) by following the procedure in *Step 1* and *Step 2*. Thus, (5.81) yields $\int_Q \frac{|\nabla\bar w_\tau|^2}{(1+\bar w)^{1+a}}\,\mathrm{d}x\,\mathrm{d}t$ bounded. Combining it with (5.49) like in (Boccardo et al., 1997; Boccardo and Galloët, 1989), cf. also (Roubíček, 2010, Formulae (4.29)-(4.33)), we obtain (5.50).

Step 4: "Dual" estimate for the time derivative:
Notice that

$$\begin{aligned}
\big\|\dot w_{\varepsilon,\tau}\big\|_{\mathcal{M}([0,T],W^{1,\infty}(\Omega)^*)} &= \sum_{k=1}^{N}\sup_{v\in W^{1,\infty},(\Omega),\,\|v\|\le1}\int_\Omega \frac{w^k_{\varepsilon,\tau}-w^{k-1}_{\varepsilon,\tau}}{\tau}v\,\mathrm{d}x\\
&= \sum_{k=1}^{N}\sup_{v\in W^{1,\infty}(\Omega),\,\|v\|\le1}\int_\Omega\Big(-\mathcal{K}(\lambda^k_{\varepsilon,\tau},w^k_{\varepsilon,\tau})\nabla w^k_{\varepsilon,\tau}\cdot\nabla v+\delta_S^*(\dot\lambda_{\varepsilon,\tau}(t_k))v+\epsilon|\dot\lambda_{\varepsilon,\tau}(t_k)|^q v\\
&\qquad+\Theta(w^k)\vec a\cdot\dot\lambda_{\varepsilon,\tau}(t_k)v\Big)\,\mathrm{d}x+\int_\Gamma(\bar b_{\varepsilon,\tau}\bar\theta_{\mathrm{ext},\varepsilon,\tau}-\bar b_{\varepsilon,\tau}\Theta(w^k_{\varepsilon,\tau}))v\,\mathrm{d}S\\
&\le \sup_{\tilde v\in C([0,T],W^{1,\infty}(\Omega)),\,\|v\|\le1}\int_Q\Big(-\mathcal{K}(\bar\lambda_{\varepsilon,\tau},\bar w_{\varepsilon,\tau})\nabla\bar w_{\varepsilon,\tau}\cdot\nabla\tilde v+\delta_S^*(\dot\lambda_{\varepsilon,\tau})\tilde v\\
&\qquad+\epsilon|\dot\lambda_{\varepsilon,\tau}|^q\tilde v\Theta(\bar w_{\varepsilon,\tau})\vec a\cdot\dot\lambda_{\varepsilon,\tau}\tilde v\Big)\,\mathrm{d}x+\int_\Gamma(\bar b_{\varepsilon,\tau}\bar\theta_{\mathrm{ext},\varepsilon,\tau}-\bar b_{\varepsilon,\tau}\Theta(\bar w_{\varepsilon,\tau}))\tilde v\,\mathrm{d}S\,\mathrm{d}t.
\end{aligned}$$

Now, because of all the preceding steps, we may use the Hölder's/Young's inequality for all terms on the right-hand side to get estimate (5.51). □

5.4.3 Convergence towards the mesoscopic model

Once the existence of microscopic solutions has established, we are in the position to prove the main theorem of this Subsection:

Theorem 5.12 (Reaching mesoscopic solutions)**.** *Let (A1)–(A7) hold and let $(y_\varepsilon, \lambda_\varepsilon, w_\varepsilon)$ be any weak solution to the microscopic system (5.28) together with initial conditions (5.29) in accord with Definition 5.7 satisfying also (5.35)–(5.39). Let also the initial conditions (5.29) be compatible with (5.18) in the sense that $\lambda_{0,\varepsilon}\to\lambda_0$ strongly in $L^q(\Omega)$, $w_{0,\varepsilon}\to w_0$ strongly in $L^1(\Omega)$ and $\nabla y_{0,\varepsilon}$ generates the family $\{[\nu_0]_x\}_{x\in\Omega}$ when $\varepsilon\to0$.*

1. *Then there exist $(y,\nu,\lambda,w)\in B([0,T];W^{1,p}(\Omega;\mathbb{R}^d))\times(\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d}))^{[0,T]}\times W^{1,q}([0,T];L^q(\Omega;\mathbb{R}^{M+1}))\times L^r([0,T];W^{1,r}(\Omega))$ and a sequence $\varepsilon\to0$ such that*

$$\lambda_\varepsilon\to\lambda \qquad \text{in } W^{1,q}(0,T;L^q(\Omega;\mathbb{R}^{M+1})), \tag{5.82}$$
$$\lambda_\varepsilon(t)\rightharpoonup\lambda(t) \qquad \text{in } L^q(\Omega;\mathbb{R}^{M+1}) \text{ for all } t\in[0,T], \tag{5.83}$$
$$w_\varepsilon\rightharpoonup w \qquad \text{in } L^r([0,T];W^{1,r}(\Omega)),\ r<\tfrac{d+2}{d+1} \tag{5.84}$$
$$w_\varepsilon\to w \qquad \text{in } L^s(Q),\ s<\frac{d+2}{d}. \tag{5.85}$$

Moreover, for each $t\in[0,T]$, there exists a subsequence $\varepsilon_{k(t)}$ such that $\nabla y_{\varepsilon_{k(t)}}(t)$ generates a family of gradient Young measures $\{\nu_x(t)\}_{x\in\Omega}$ and $y_{\varepsilon_{k(t)}}(t)\rightharpoonup y(t)$ in $W^{1,p}(\Omega;\mathbb{R}^d)$.

2. *At least one cluster point* (y,ν,λ,w) *obtained in this way is a weak solution of* (5.17) *in accord with Definition* 5.4*, and thus, in particular, such solutions do exist.*

Proof. The proof was given (Benešová and Roubíček, 2012) (obtained within the work on this thesis) – we reprint it here for the readers' convenience – and is similar to the convergence part of proof Proposition 5.9. However; it is rather peculiar to find a cluster-point (y,ν,λ,w) that fulfills (5.23) – the main difficulty is due to the term $\int_0^T\int_\Omega \mathcal{Q}'_\varkappa(\lambda-L\bullet\nu)\cdot(v-\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t$. In particular, it is non-trivial to assure measurability of the integrand since $\nu(t)$ (as obtained in point 1 of Theorem 5.12) *needs not be measurable itself.*

Therefore, we use (5.31), to reformulate (5.33) into a yet weaker form, which we call the *reformulated microscopic flow-rule*. In this weaker form, a part of the problematic term, namely $\int_0^T \mathcal{Q}'_\varkappa(\lambda-L\bullet\nu)\cdot\dot\lambda\,\mathrm{d}x\,\mathrm{d}t$, is not present anymore (cf. *Step 1*). Nevertheless, the second part $\int_0^T \mathcal{Q}'_\varkappa(\lambda-L\bullet\nu)\cdot v\,\mathrm{d}x\,\mathrm{d}t$ cannot be removed, so the measurability problem is not solved just by this reformulation.

Hence, we use a technique based on Fatou's lemma (Dal Maso et al., 2005; Francfort and Mielke, 2006) to select a cluster point for which the above integral makes sense; note however that we can only show that the *whole above integrand is measurable, not the cluster point itself* (cf. *Step 2*).

For lucidity, let us again divide the proof into several steps.

Step 1: Selection of subsequences, reformulated flow-rule and limit passage in it
By the same procedure as in *Step 3* of the proof Proposition 5.9 we can, owing to (5.35)–(5.39), find a subsequence of ε's (not relabeled) and (λ,w) such that

$$\lambda_\varepsilon \overset{*}{\rightharpoonup} \lambda \quad \text{in } W^{1,q}([0,T];L^q(\Omega;\mathbb{R}^{M+1})) \tag{5.86}$$

and (5.83) - (5.85) hold; note that (5.85) also assures that $\Theta(w_\varepsilon)\to\Theta(w)$ in $L^{q'}(Q)$.[24]

Next, let us reformulate the flow-rule (5.33) into a weaker form using the mechanical energy inequality (5.31).[25] To do so, let us first *abbreviate*

$$\mathfrak{G}_\varepsilon(T)=\mathfrak{G}_\varepsilon(T,y_\varepsilon(T),\lambda_\varepsilon(T)) \qquad \text{and} \qquad \mathfrak{G}_\varepsilon(0)=\mathfrak{G}_\varepsilon(0,y_\varepsilon(0),\lambda_\varepsilon(0)).$$

Thus, we recall that (5.31) states that

$$-\int_Q \mathcal{P}_\varkappa(\lambda_\varepsilon,\nabla y_\varepsilon)\dot\lambda_\varepsilon\,\mathrm{d}x\,\mathrm{d}t=\mathfrak{G}_\varepsilon(0)-\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T])-\mathfrak{G}_\varepsilon(T)+\int_0^T[\mathfrak{G}'_\varepsilon]_t(t,y_\varepsilon(t))\,\mathrm{d}t.$$

By plugging this into (5.33), we get the following *reformulated flow rule*:

$$\begin{aligned}\int_Q \rho_q(\dot\lambda_\varepsilon)\,\mathrm{d}x\,\mathrm{d}t \le \int_Q \rho_q(v)+(\Theta(w_\varepsilon)-\theta_{\mathrm{tr}})(v-\dot\lambda_\varepsilon)+\mathcal{P}_\varkappa(\lambda_\varepsilon,\nabla y_\varepsilon)v\,\mathrm{d}x\,\mathrm{d}t\\ +\mathfrak{G}_\varepsilon(0)-\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T])-\mathfrak{G}_\varepsilon(T)+\int_0^T[\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon(t))\,\mathrm{d}t.\end{aligned} \tag{5.87}$$

Let us now pass to the limit $\varepsilon\to 0$ in (5.87). Here, the terms $\int_Q \mathcal{P}_\varkappa(\lambda_\varepsilon,\nabla y_\varepsilon)v\,\mathrm{d}x\,\mathrm{d}t$ and $[\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon(t))$ turn out to be the most difficult ones because a-priori estimate (5.35)

[24] Indeed, thanks to the growth condition $|\Theta(w)|\le C(1+|w|^{1/\omega})$ and $\omega>q'$ (cf. assumption (A4)), we have that $|\Theta(w)|\le C(1+|w|^{1/\omega})\le C(1+|w|^{1/q'})$. Hence, applying the continuity of Nemytskii mapping induced by Θ, we have the claim.

[25] We use this procedure to cope with the aforementioned problems with measurability of $\int_0^T\int_\Omega \mathcal{Q}'_\varkappa(\lambda-L\bullet\nu)\cdot(v-\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t$.

directly implies only $y_\varepsilon \overset{*}{\rightharpoonup} y$ in $L^\infty([0,T];W^{1,p}(\Omega;\mathbb{R}^d))$ which would not be sufficient for the limit passage due to involved the non-linearities. We shall circumpass this problem using a trick inspired by (Dal Maso et al., 2005) or (Francfort and Mielke, 2006, Section 3, Step 2).

First, however, we establish the convergence of all other terms. Using weak lower semi-continuity properties for the convex term ρ_q on the left-hand side of (5.87), we get that $\int_Q \rho_q(\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t \le \liminf_{\varepsilon\to 0}\int_Q \rho_q(\dot\lambda_\varepsilon)\,\mathrm{d}x\,\mathrm{d}t$, similarly as in *Step 4* of the proof Proposition 5.9. On the right-hand side of (5.87), we can use that $\Theta(w_\varepsilon)\to\Theta(w)$ in $L^{q'}(Q)$ (established in Step 1) to pass to the limit in $\int_Q \Theta((w_\varepsilon)-\theta_{\mathrm{tr}})(v-\dot\lambda_\varepsilon)\,\mathrm{d}x\,\mathrm{d}t$. Moreover, $\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T])$ is non-negative and can be omitted. Eventually, as $\mathfrak{G}_\varepsilon(0)$ and $\mathfrak{G}_\varepsilon(T)$ are bounded sequences of numbers, we may assume that $\lim_{\varepsilon\to 0}\mathfrak{G}_\varepsilon(0)$ and $\lim_{\varepsilon\to 0}\mathfrak{G}_\varepsilon(T)$ exist – for if they did not, we could always find a sub-sequence of ε in which the convergences would hold and then work only with this subsequence. We shall identify these limits in *Step 2*.

Let us choose a *fixed test function* $v\in\mathcal{V}$, where $\mathcal{V}$ is a countable dense subset of $L^q([0,T];L^q(\Omega;\mathbb{R}^{M+1}))$ and turn to the difficult terms $\int_Q \mathcal{P}_\varkappa(\lambda_\varepsilon,\nabla y_\varepsilon)v\,\mathrm{d}x\,\mathrm{d}t$ and $[\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon(t))$. We define the functions $\mathcal{L}^v$, dependent on the choice of the test function v, and $\mathcal{F}$ by

$$\mathcal{L}^v(t)=\limsup_{\varepsilon\to 0}\int_\Omega \mathcal{P}_\varkappa(\lambda_\varepsilon(t),\nabla y_\varepsilon(t))v(t)\,\mathrm{d}x,\quad \mathcal{F}(t)=\limsup_{\varepsilon\to 0}[\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon(t)). \tag{5.88}$$

Since $\int_\Omega \mathcal{P}_\varkappa(\lambda_\varepsilon(t),\nabla y_\varepsilon(t))v(t)\,\mathrm{d}x$ as well as $[\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon(t))$ are bounded from above by measurable functions, thanks to estimates (5.35) and (5.36), Fatou's lemma gives that both $\mathcal{L}^v$ and $\mathcal{F}$ are measurable and

$$\limsup_{\varepsilon\to 0}\int_Q \mathcal{P}_\varkappa(\lambda_\varepsilon,\nabla y_\varepsilon)v\,\mathrm{d}x\,\mathrm{d}t\le\int_0^T\mathcal{L}^v\,\mathrm{d}t,\qquad \limsup_{\varepsilon\to 0}\int_0^T[\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon(t))\,\mathrm{d}t\le\int_0^T\mathcal{F}\,\mathrm{d}t.$$

Plugging the above estimates into (5.87) leads to

$$\begin{aligned}
\int_Q\rho_q(\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t&\le\liminf_{\varepsilon\to 0}\int_Q\rho_q(\dot\lambda_\varepsilon)\,\mathrm{d}x\,\mathrm{d}t\\
&\le\liminf_{\varepsilon\to 0}\int_0^T\Big([\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon)+\int_\Omega\mathcal{P}_\varkappa(\lambda_\varepsilon,\nabla y_\varepsilon)v+(\Theta(w_\varepsilon)-\theta_{\mathrm{tr}})(v-\dot\lambda_\varepsilon)+\rho_q(v)\,\mathrm{d}x\Big)\,\mathrm{d}t\\
&\qquad+\mathfrak{G}_\varepsilon(0)-\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;[0,T])-\mathfrak{G}_\varepsilon(T)\\
&\le\limsup_{\varepsilon\to 0}\int_0^T\Big([\mathfrak{G}_\varepsilon]'_t(t,y_\varepsilon)+\int_\Omega\mathcal{P}_\varkappa(\lambda_\varepsilon,\nabla y_\varepsilon)v+(\Theta(w_\varepsilon)-\theta_{\mathrm{tr}})(v-\dot\lambda_\varepsilon)+\rho_q(v)\,\mathrm{d}x\Big)\,\mathrm{d}t\\
&\qquad+\mathfrak{G}_\varepsilon(0)-\mathfrak{G}_\varepsilon(T)\\
&\le\int_0^T\mathcal{L}^v+\mathcal{F}\,\mathrm{d}t+\int_Q(\Theta(w)-\theta_{\mathrm{tr}})(v-\dot\lambda)+\rho_q(v)\,\mathrm{d}x\,\mathrm{d}t+\lim_{\varepsilon\to 0}\mathfrak{G}_\varepsilon(0)-\lim_{\varepsilon\to 0}\mathfrak{G}_\varepsilon(T).
\end{aligned}\tag{5.89}$$

Now we take $t\in[0,T]$ arbitrary but fixed. Then, for any $v\in\mathcal{V}$, we may find a t-dependent subsequence of ε's, denoted as $\varepsilon_{k(t,v)}$, such that

$$\mathcal{L}^v(t)=\lim_{\varepsilon_{k(t,v)}\to 0}\int_\Omega\mathcal{P}_\varkappa(\lambda_{\varepsilon_{k(t,v)}}(t),\nabla y_{\varepsilon_{k(t,v)}}(t))v(t)\,\mathrm{d}x, \tag{5.90}$$

$$\mathcal{F}(t)=\lim_{\varepsilon_{k(t,v)}\to 0}[\mathfrak{G}_\varepsilon]'_t(t,y_{\varepsilon_{k(t,v)}}(t)). \tag{5.91}$$

By a diagonal selection, we can find a further (still time-dependent) subsequence labeled $\varepsilon_{k(t)}$, such that (5.90)–(5.91) hold *even for all* v from the countable set $\mathcal{V}$.

Using the second estimate in (5.35) we may again select a subsequence of $\varepsilon_{k(t)}$ (not relabeled) such that $y_{\varepsilon_{k(t)}}(t)\rightharpoonup y(t)$ weakly in $W^{1,p}(\Omega;\mathbb{R}^d)$ and $\nabla y_{\varepsilon_{k(t)}}$ generates a

family of Young measures $\nu(t) \in \mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^{d\times d})$ with $\mathrm{id}\bullet\nu_x(t) = \nabla y(x,t)$ a.e. on Ω. Then, because L is bounded, $L(\nabla y_{\varepsilon_{k(t)}}(t)) \to L\bullet\nu(t)$ weakly* in $L^\infty(\Omega)$. Combining this with (5.83) and (5.2), gives that $\mathcal{P}_\varkappa(\lambda_\varepsilon(t),\nabla y_\varepsilon(t)) \to \mathcal{Q}'_\varkappa(\lambda(t)-L\bullet\nu(t))$ in $L^2(\Omega)$. Therefore, (5.90) and (5.91) yield

$$\mathcal{L}^v(t) = \lim_{\varepsilon_{k(t)}\to 0}\int_\Omega \mathcal{P}_\varkappa(\lambda_{\varepsilon_{k(t)}}(t),\nabla y_{\varepsilon_{k(t)(t)}})v(t)\,\mathrm{d}x = \int_\Omega \mathcal{Q}'_\varkappa(\lambda(t)-L\bullet\nu(t))v(t)\,\mathrm{d}x,$$
$$\mathcal{F}(t) = \lim_{\varepsilon_{k(t)}\to 0}[\mathfrak{G}_\varepsilon]'_t(t,y_{\varepsilon_{k(t)}}(t)) = \int_\Omega f(t)\cdot y(t)\,\mathrm{d}x + \int_{\Gamma_N} g(t)\cdot y(t)\,\mathrm{d}S,$$

for all $v\in\mathcal{V}$. This holds even for all $t\in[0,T]$, since t, chosen above, was arbitrary. Inserting this into (5.89) finally leads to

$$\int_Q \rho_q(\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t \le \int_0^T\int_\Omega \Big(\mathcal{Q}'_\varkappa(\lambda-L\bullet\nu)v + f\cdot y\,\mathrm{d}x + \int_{\Gamma_N} g\cdot y\,\mathrm{d}S\Big)\,\mathrm{d}t$$
$$+ \lim_{\varepsilon\to 0}\mathfrak{G}_\varepsilon(0) - \lim_{\varepsilon\to 0}\mathfrak{G}_\varepsilon(T) + \int_Q(\Theta(w)-\theta_{\mathrm{tr}})(v-\dot\lambda) + \rho_q(v)\,\mathrm{d}x\,\mathrm{d}t. \tag{5.92}$$

for all $v\in\mathcal{V}$. This can be extended for any $v\in L^q(Q)$ by continuity. Note that the measurability of $\mathcal{Q}'_\varkappa(\lambda-L\bullet\nu)v$ is guaranteed for any $v\in L^q(Q;\mathbb{R}^{M+1})$ since for a.e. $x\in\Omega$ and a.e. $t\in[0,T]$ $\mathcal{Q}'_\varkappa(\lambda(x,t)-L\bullet\nu_x(t))v(x,t)$ is the limit of $\mathcal{Q}'_\varkappa(\lambda(x,t)-L\bullet\nu_x(t))v_k(x,t)$ with $v_k\in\mathcal{V}$.

Step 2: Limiting the minimization principle
In this step we show that (5.22) holds. To shorten the notation, we first introduce, in analogy to the microscopic case (5.32), the *mechanical part of the Gibbs free energy*:

$$\mathfrak{G}(t,y,\nu,\lambda) = \int_\Omega \phi_1\bullet\nu - f(t)\cdot y\,\mathrm{d}x - \int_{\Gamma_N} g(t)\cdot y\,\mathrm{d}S + \mathcal{Q}_\varkappa(\lambda-L\bullet\nu); \tag{5.93}$$

with this notation, (5.22) is equivalent to

$$\mathfrak{G}(t,y(t),\nu(t),\lambda(t)) \le \mathfrak{G}(t,\tilde y,\tilde\nu,\lambda(t))$$

for any couple $(\tilde y,\tilde\nu)\in W^{1,p}(\Omega;\mathbb{R}^d)\times\mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^{d\times d})$ such that $\nabla\tilde y(x) = \mathrm{id}\bullet\tilde\nu_x$ for a.a. $x\in\Omega$ and all $t\in[0,T]$.

Again, we take some $t\in[0,T]$ arbitrary but fixed. Since the specific stored energy is bounded from below (cf. assumption (A1)) we have that $\int_\Omega \phi_1\bullet\nu(t)\,\mathrm{d}x \le \liminf_{\varepsilon_{k(t)}\to 0}\int_\Omega \phi_1(\nabla y_{\varepsilon_{k(t)}}(t))\,\mathrm{d}x$, cf. (Pedregal, 1997). Moreover, by exploiting the minimization principle (5.30)[26], we may write

$$\mathfrak{G}(t,y(t),\nu(t),\lambda(t)) \le \liminf_{\varepsilon_{k(t)}\to 0}\mathfrak{G}_{\varepsilon_{k(t)}}(t,y_{\varepsilon_{k(t)}}(t),\lambda_{\varepsilon_{k(t)}}(t))$$
$$\le \liminf_{\varepsilon_{k(t)}\to 0}\mathfrak{G}_{\varepsilon_{k(t)}}(t,\tilde y,\lambda_{\varepsilon_{k(t)}}(t)) + \int_\Omega \varepsilon_{k(t)}|\nabla\tilde y - \nabla y_{\varepsilon_{k(t)}}(t)|\,\mathrm{d}x$$
$$= \int_\Omega \phi_1(\nabla\tilde y(t)) - f(t)\cdot\tilde y\,\mathrm{d}x + \mathcal{Q}_\varkappa(\lambda(t)-L(\nabla\tilde y(t))) - \int_{\Gamma_N} g(t)\cdot\tilde y\,\mathrm{d}S, \tag{5.94}$$

for any $\tilde y\in W^{2,2}(\Omega;\mathbb{R}^d)$. In the last equality, we used that $\nabla y_{\varepsilon_{k(t)}}(t)$ is bounded in $L^1(\Omega;\mathbb{R}^{d\times d})$ independently of ε (cf. (5.35), line 2) and hence $\int_\Omega \varepsilon_{k(t)}|\nabla\tilde y - \nabla y_{\varepsilon_{k(t)}}(t)|\,\mathrm{d}x \to 0$ as $\varepsilon\to 0$. Realizing that $W^{2,2}(\Omega;\mathbb{R}^d)$ is dense in $W^{1,p}(\Omega;\mathbb{R}^d)$, from (5.94) we have

[26] Although we proceed here analogously to the proof Proposition 4.1, for clarity, a detailed proof is given here, too.

$$\mathfrak{G}(t,y(t),\nu(t),\lambda(t)) \le \int_\Omega \phi_1(\nabla\tilde y)-f(t)\cdot\tilde y\,\mathrm{d}x+\mathcal{Q}_\varkappa(L(\lambda(t)-\nabla\tilde y))-\int_{\Gamma_{\rm N}} g(t)\cdot\tilde y\,\mathrm{d}S, \quad (5.95)$$

even for any $\tilde y \in W^{1,p}(\Omega;\mathbb{R}^d)$.

Take any $\hat\nu \in \mathscr{G}^p_{\Gamma_{\rm D}}(\Omega;\mathbb{R}^{d\times d})$ and its generating sequence $\{\hat y_k\}_{k=1}^\infty$ such that $\{|\nabla\hat y_k|^p\}_{k=1}^\infty$ is equi-integrable; recall, from Chapter 2, that taking such an equi-integrable generating sequence implies that $\phi_1(\nabla\tilde y) \rightharpoonup \phi_1\bullet\nu$ in $L^1(\Omega)$, even though ϕ_1 is of p-growth. We now plug $\hat y_k$ into (5.95) in place of $\tilde y$, and let $k\to\infty$ to obtain

$$\mathfrak{G}(t,y(t),\nu(t),\lambda(t)) \le \int_\Omega \phi_1\bullet\hat\nu-f(t)\cdot\hat y\,\mathrm{d}x+\mathcal{Q}_\varkappa(\lambda(t)-L\bullet\hat\nu)-\int_{\Gamma_{\rm N}} g(t)\cdot\hat y\,\mathrm{d}S = \mathfrak{G}(t,\hat y,\hat\nu,\lambda(t)),$$

with $\hat y$ the weak limit of $\{\hat y_k\}_{k=1}^\infty$ in $W^{1,p}(\Omega;\mathbb{R}^d)$ giving the desired minimization principle (5.22). Note that, for $(\hat y,\hat\nu)=(y(t),\nu(t))$, this procedure also gives $\mathfrak{G}(t,y(t),\nu(t),\lambda(t))$ $=\lim_{\varepsilon_{k(t)}\to0}\mathfrak{G}_{\varepsilon_{k(t)}}(t,y_{\varepsilon_{k(t)}}(t),\lambda_{\varepsilon_{k(t)}}(t))$, which in particular means that

$$\begin{cases} \mathfrak{G}(0)\equiv\mathfrak{G}(0,y(0),\nu(0),\lambda(0))=\lim_{\varepsilon\to0}\mathfrak{G}_\varepsilon(0),\\ \mathfrak{G}(T)\equiv\mathfrak{G}(T,y(T),\nu(T),\lambda(T))=\lim_{\varepsilon\to0}\mathfrak{G}_\varepsilon(T).\end{cases} \quad (5.96)$$

Step 3: Reverse energy inequality, strong convergence of $\dot\lambda$, back to the original flow-rule As a corollary of the minimization principle (5.22), we can prove, analogously to *Step 6* of the proof Proposition 5.9 the following the mechanic energy inequality

$$\mathfrak{G}(0)-\mathfrak{G}(T)+\int_0^T \mathfrak{G}'_t(t,y(t))\,\mathrm{d}t \le -\int_Q \mathcal{Q}_\varkappa(\lambda-L\bullet\nu)\dot\lambda\,\mathrm{d}x\,\mathrm{d}t. \quad (5.97)$$

Indeed, any partition $0=t_0^\beta<t_1^\beta<\ldots<t_k^\beta=T$ with $\max_{i=1,\ldots,k}(t_i^\beta-t_{i-1}^\beta)\le\beta$ of the interval $[0,T]$, it holds that

$$\begin{aligned}\mathfrak{G}(t_{i-1}^\beta,&y(t_{i-1}^\beta),\nu(t_{i-1}^\beta),\lambda(t_{i-1}^\beta)) \le \mathfrak{G}(t_{i-1}^\beta,y(t_i^\beta),\nu(t_i^\beta),\lambda(t_{i-1}^\beta))\\ &=\mathfrak{G}(t_i^\beta,y(t_i^\beta),\nu(t_i^\beta),\lambda(t_i^\beta))-\int_{t_{i-1}^\beta}^{t_i^\beta}\mathfrak{G}'_t(t,y(t_i^\beta))+\langle\mathfrak{G}'_\lambda(\nu(t_i^\beta),\lambda(t)),\dot\lambda(t)\rangle\,\mathrm{d}t\end{aligned}$$

where the first inequality is due to (5.22) and where we used that $\mathfrak{G}'_t$ is independent of ν and λ while $\mathfrak{G}'_\lambda$ is independent of t and y. Summing this expression for $i=1,...,k$ leads to

$$\begin{aligned}\mathfrak{G}(T)-\mathfrak{G}(0) &\ge \sum_{i=1}^k\int_{t_{i-1}^\beta}^{t_i^\beta}\mathfrak{G}'_t(t,y(t_i^\beta))+\int_\Omega\mathcal{Q}'_\varkappa(\lambda(t)-L\bullet\nu(t_i^\beta))\dot\lambda(t)\,\mathrm{d}t\\ &=\sum_{i=1}^k\int_{t_{i-1}^\beta}^{t_i^\beta}\Big(\int_\Omega\underbrace{\mathcal{Q}'_\varkappa(\lambda(t)-\lambda(t_i^\beta))\cdot\dot\lambda(t)}_{=S_1}+\underbrace{\mathcal{Q}'_\varkappa(\lambda(t_i^\beta)-L\bullet\nu(t_i^\beta))\cdot\dot\lambda(t_i^\beta)}_{=S_2}\,\mathrm{d}x\\ &\quad+\int_\Omega\underbrace{\mathcal{Q}'_\varkappa(\lambda(t_i^\beta)-L\bullet\nu(t_i^\beta))\cdot(\dot\lambda(t)-\dot\lambda(t_i^\beta))}_{=S_3}\,\mathrm{d}x+\underbrace{\mathfrak{G}'_t(t,y(t_i^\beta))}_{=S_4}\Big)\,\mathrm{d}t, \quad (5.98)\end{aligned}$$

where we can pass to the limit in S_1, S_2, S_3 and S_4 the same way as in (5.72), (5.71), (5.73) and (5.70), respectively to obtain (5.97).

Let us now exploit (5.97) to prove that $\dot\lambda_\varepsilon\to\dot\lambda$ *strongly* in $L^q(Q;\mathbb{R}^{M+1})$; analogously to *Step 5* of the proof Proposition 5.9. To this end, let us first approximate $\dot\lambda$ by some $\{\lambda'_j\}_{j\in\mathbb{N}}\subset\mathcal{V}$ with $\mathcal{V}$ the dense countable subset of $L^q(Q;\mathbb{R}^{M+1})$ used already in *Step 1*,

i.e. $\lambda_j' \to \dot\lambda$ in $L^q(Q)$ as $j\to\infty$. Such an approximation shall be needed since, following *Step 1*, we only know that $\limsup_{\varepsilon\to0}\int_Q \mathcal{P}_\varkappa(\lambda_\varepsilon,\nabla y_\varepsilon)v\,\mathrm{d}x \le \int_Q \mathcal{Q}'_\varkappa(\lambda{-}L\bullet\nu)v\,\mathrm{d}x$ for $v\in\mathcal{V}$; hence we can assure this inequality for $v=\lambda_j'$ but not for $v=\dot\lambda$.

As in *Step 5* of the proof Proposition 5.9, we test the reformulated microscopic flow-rule (5.87), here *once again rewritten using the convexity of* $|\cdot|^q$, by $v=\lambda_j'$. This yields

$$\int_Q \delta_S^*(\dot\lambda_\varepsilon)\,\mathrm{d}x\,\mathrm{d}t \le \int_0^T\Big([\mathfrak{G}_\varepsilon]_t'(t,y_\varepsilon)+\int_\Omega \mathcal{P}_\varkappa(\lambda_\varepsilon,\nabla y_\varepsilon)\lambda_j'+\alpha|\dot\lambda_\varepsilon|^{q-2}\dot\lambda_\varepsilon(\lambda_j'-\dot\lambda_\varepsilon) \\ +(\Theta(w_\varepsilon){-}\theta_{\mathrm{tr}})(\lambda_j'{-}\dot\lambda_\varepsilon)+\delta_S^*(\lambda_j')\,\mathrm{d}x\Big)\,\mathrm{d}t-\mathfrak{G}_\varepsilon(T)+\mathfrak{G}_\varepsilon(0). \tag{5.99}$$

Symmetrically, we test (5.92) (the reformulated limited flow-rule; here again rewritten using the convexity of $|\cdot|^q$ and also (5.96)) by $v=\dot\lambda_\varepsilon$ to get

$$\int_Q \delta_S^*(\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t \le \int_0^T\Big(\mathfrak{G}_t'(t,y)+\int_\Omega \mathcal{Q}'_\varkappa(\lambda{-}L\bullet\nu)\dot\lambda_\varepsilon+\alpha|\dot\lambda|^{q-2}\dot\lambda(\dot\lambda_\varepsilon{-}\dot\lambda) \\ +(\Theta(w){-}\theta_{\mathrm{tr}})(\dot\lambda_\varepsilon{-}\dot\lambda)+\delta_S^*(\dot\lambda_\varepsilon)\,\mathrm{d}x\Big)\,\mathrm{d}t-\mathfrak{G}(T)+\mathfrak{G}(0). \tag{5.100}$$

Add (5.99) and (5.100) and apply $\limsup_{\varepsilon\to0}$ to get

$$\begin{aligned}
&\alpha\lim_{\varepsilon\to0}\Big(\|\dot\lambda_\varepsilon\|_{L^q(Q)}^{q-1}{-}\|\dot\lambda\|_{L^q(Q)}^{q-1}\Big)\Big(\|\dot\lambda_\varepsilon\|_{L^q(Q)}{-}\|\dot\lambda\|_{L^q(Q)}\Big)\\
&\quad\le\limsup_{\varepsilon\to0}\ \alpha\int_Q\Big(|\dot\lambda_\varepsilon|^{q-2}\dot\lambda_\varepsilon{-}|\dot\lambda|^{q-2}\dot\lambda\Big)\cdot(\dot\lambda_\varepsilon{-}\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t\\
&\quad\le\limsup_{\varepsilon\to0}\Big(\mathfrak{G}(0){-}\mathfrak{G}(T){+}\underbrace{\mathfrak{G}_\varepsilon(0){-}\mathfrak{G}_\varepsilon(T)}_{\text{(I)}}+\int_0^T\mathfrak{G}_t'(t,y){+}\underbrace{[\mathfrak{G}_\varepsilon]_t'(t,y_\varepsilon)}_{\text{(II)}}\\
&\qquad+\int_\Omega\alpha\underbrace{|\dot\lambda_\varepsilon|^{q-2}\dot\lambda_\varepsilon(\lambda_j'{-}\dot\lambda)}_{\text{(III)}}{+}\delta_S^*(\lambda_j'){-}\delta_S^*(\dot\lambda)\,\mathrm{d}x{+}\underbrace{\mathcal{P}_\varkappa(\lambda_\varepsilon,\nabla y_\varepsilon)(\lambda_j')}_{\text{(IV)}}+\underbrace{\mathcal{Q}'_\varkappa(\lambda{-}L\bullet\nu)\dot\lambda_\varepsilon}_{\text{(V)}}\\
&\qquad+\underbrace{(\Theta(w_\varepsilon){-}\theta_{\mathrm{tr}})(\lambda_j'{-}\dot\lambda_\varepsilon){+}(\Theta(w){-}\theta_{\mathrm{tr}})(\dot\lambda_\varepsilon{-}\dot\lambda)}_{\text{(VI)}}\,\mathrm{d}x\,\mathrm{d}t\Big)\\
&\quad\le C\|\lambda_j'{-}\dot\lambda\|_{L^q(Q)}+\int_Q\delta_S^*(\lambda_j'){-}\delta_S^*(\dot\lambda){+}(\Theta(w){-}\theta_{\mathrm{tr}})(\lambda_j'{-}\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t\\
&\qquad+\int_0^T\Big(\int_\Omega\mathcal{Q}'_\varkappa(\lambda{-}L\bullet\nu)(\lambda_j'{+}\dot\lambda)\,\mathrm{d}x{+}2\mathfrak{G}_t'(t,y)\Big)\,\mathrm{d}t-2\mathfrak{G}(T)+2\mathfrak{G}(0).
\end{aligned}\tag{5.101}$$

We used in (5.101) that Term (I) converges to $\mathfrak{G}(T){+}\mathfrak{G}(0)$ by *Step 2*, cf. (5.96) whereas Term (II) is, owing to *Step 1*, bounded from above by $\mathfrak{G}_t'(t,y)$. Further we exploited for Term (III) that $\dot\lambda_\varepsilon$ is bounded in $L^q(Q;\mathbb{R}^{M+1})$. The limsup of Term (IV) is, by *Step 1*, bounded from above by $\int_\Omega\mathcal{Q}'_\varkappa(\lambda{-}L\bullet\nu)\lambda_j'\,\mathrm{d}x$; for Term (V) we used only the weak convergence of $\dot\lambda_\varepsilon$ in $L^q(Q;\mathbb{R}^{M+1})$. For Term (VI) we again exploited the weak convergence of $\dot\lambda_\varepsilon$ in $L^q(Q;\mathbb{R}^{M+1})$ and the fact that $\Theta(w_\varepsilon)\to\Theta(w)$ strongly in $L^{q'}(Q)$ (cf. *Step 1*). Letting now $j\to\infty$ leads to

$$
\begin{aligned}
&\alpha \lim_{\varepsilon\to 0}\Big(\|\dot\lambda_\varepsilon\|_{L^q(Q)}^{q-1}-\|\dot\lambda\|_{L^q(Q)}^{q-1}\Big)\Big(\|\dot\lambda_\varepsilon\|_{L^q(Q)}-\|\dot\lambda\|_{L^q(Q)}\Big)\\
&\quad\le \lim_{j\to\infty}\Big(C\|\lambda_j'-\dot\lambda\|_{L^Q(Q)}+\int_Q \delta_S^*(\lambda_j')-\delta_S^*(\dot\lambda)+(\Theta(w)-\theta_{\rm tr})(\lambda_j'-\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t\\
&\qquad+\int_0^T\Big(\int_\Omega \mathcal{Q}_\varkappa'(\lambda-L\bullet\nu)(\lambda_j'+\dot\lambda)\,\mathrm{d}x+2\mathfrak{G}_t'(t,y)\Big)\,\mathrm{d}t-2\mathfrak{G}(T)+2\mathfrak{G}(0)\Big)\\
&\quad\le 2\left(\int_0^T\Big(\int_\Omega \mathcal{Q}_\varkappa'(\lambda-L\bullet\nu)\dot\lambda\,\mathrm{d}x+\mathfrak{G}_t'(t,y)\Big)\,\mathrm{d}t-\mathfrak{G}(T)+\mathfrak{G}(0)\right)\le 0,
\end{aligned}
$$

by (5.97). Hence, we obtained $\|\dot\lambda_\varepsilon\|_{L^q(Q)}\to\|\dot\lambda\|_{L^q(Q)}$, and from (5.86) by the uniform convexity of the norm of $L^q(Q)$, we obtain $\dot\lambda_\varepsilon\to\dot\lambda$ strongly, i.e. (5.82).

Finally, notice that plugging (5.97) into (5.92) indeed gives (5.17b)

Step 4: Limiting the enthalpy equation
In order to pass to the limit $\varepsilon\to 0$ in the enthalpy equation (5.34), we first show that $\varepsilon\int_{\bar Q}\zeta\,\mathcal{H}_\varepsilon(\,\mathrm{d}x\,\mathrm{d}t)$ converges to 0; recall that $\mathcal{H}_\varepsilon$ is the measure defined by prescribing its values on every closed set $A=[t_1,t_2]\times B$, where $B\subset\Omega$ is a Borel set as

$$
\mathcal{H}_\varepsilon(A)=\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;B\times[t_1,t_2])
$$

i.e. we just need to show that $\lim_{\varepsilon\to0}\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T])=0$ since this implies $\varepsilon\int_{\bar Q}\zeta\,\mathcal{H}_\varepsilon(\,\mathrm{d}x\,\mathrm{d}t)\to0$.

To this end, we exploit the mechanical energy equality (5.31) and have that

$$
\begin{aligned}
\limsup_{\varepsilon\to0}\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T])\le\limsup_{\varepsilon\to0}\Big(&-\mathfrak{G}_\varepsilon(T)+\mathfrak{G}_\varepsilon(0)\\
&+\int_0^T\langle[\mathfrak{G}_\varepsilon]_\lambda'(y_\varepsilon(t),\lambda_\varepsilon(t)),\dot\lambda_\varepsilon\rangle+[\mathfrak{G}_\varepsilon]_t'(t,y_\varepsilon(t))\,\mathrm{d}t\Big).
\end{aligned}
\tag{5.102}
$$

To pass to the limit on the right-hand side, we rewrite $\langle[\mathfrak{G}_\varepsilon]_\lambda'(y_\varepsilon(t),\lambda_\varepsilon(t)),\dot\lambda_\varepsilon\rangle=\langle[\mathfrak{G}_\varepsilon]_\lambda'(y_\varepsilon(t),\lambda_\varepsilon(t)),\dot\lambda\rangle+\langle[\mathfrak{G}_\varepsilon]_\lambda'(y_\varepsilon(t),\lambda_\varepsilon(t)),\dot\lambda_\varepsilon-\dot\lambda\rangle$; note that for the first term we get by *Step 1* $\limsup_{\varepsilon\to0}\int_0^T\langle[\mathfrak{G}_\varepsilon]_\lambda'(y_\varepsilon(t),\lambda_\varepsilon(t)),\dot\lambda\rangle\,\mathrm{d}t\le\int_0^T\langle[\mathfrak{G}]_\lambda'(y(t),\lambda(t)),\dot\lambda\rangle\,\mathrm{d}t$ while the second term converges to 0 in $L^1([0,T])$ owing to *Step 3*. Using once again the procedure of *Step 1* for the term $[\mathfrak{G}_\varepsilon]_t'(t,y_\varepsilon(t))$ and exploiting also (5.96) we arrive at

$$
\limsup_{\varepsilon\to0}\varepsilon\mathrm{Var}_{|\cdot|}(\nabla y_\varepsilon;\Omega\times[0,T])\le\mathfrak{G}(0)+\int_0^T\langle[\mathfrak{G}]_\lambda'(\nu(t),\lambda(t)),\dot\lambda\rangle+[\mathfrak{G}]_t'(t,y(t))\,\mathrm{d}t-\mathfrak{G}(T)\le0,
$$

where the last inequality is due to (5.97). The passage in all other terms follows *Step 7* in the proof Proposition 5.9. □

5.5 Proof Theorem 5.6 via time-discretization

Although we have already proved Theorem 5.6 in the last section, here we present a different proof based on time-discretization. This is essential since such a type of proof provides instructions how to construct numerical schemes in order to guarantee convergence of discrete solutions to continuous ones.

When proving that time-discrete solution converge to (some) weak solutions of (5.17), we combine the arguments from the proof Proposition 5.9 and Theorem 5.12; in particular we exploit the ideas of Proposition 5.9 for a-priori estimates and some parts of the convergence argument, the procedure from the proof Theorem 5.12 is, on the other hand, useful to select subsequences in such a manner that $\int_0^T\!\int_\Omega\langle\mathcal{Q}_\varkappa'(\lambda-L\bullet\nu),v-\dot\lambda\rangle\,\mathrm{d}x\,\mathrm{d}t$ is meaningful.

5.5.1 Discretization by Rothe's method

Let us start by introducing a uniform partition $0 = t_0 < t_1 < t_2 \dots t_N = T$ with $(t_i - t_{i-1}) = \tau$ for $i = 1 \dots N$ of the time-interval $[0, T]$. Then, we discretize (5.17) by the backwards Euler method.

Hence, we call the quadruple $(y_\tau^k, \nu_\tau^k, \lambda_\tau^k, w_\tau^k) \in W^{1,p}_{\Gamma_{\rm D}}(\Omega;\mathbb{R}^d) \times \mathscr{G}^p_{\Gamma_{\rm D}}(\Omega;\mathbb{R}^{d\times d}) \times L^{2q}(\Omega;\mathbb{R}^{M+1}) \times W^{1,2}(\Omega)$ the *discrete weak solution* of (5.17) time-level k, $k = 1 \dots T/\tau$, if it satisfies:

1. The **minimization problem for** λ with given λ_τ^{k-1}, w_τ^{k-1}, y_τ^{k-1} and ν_τ^{k-1}:

$$\left.\begin{aligned} &\text{Minimize} \quad \mathcal{G}(k\tau, y_\tau^{k-1}, \nu_\tau^{k-1}, \lambda, \Theta(w_\tau^{k-1})) + \tau\int_\Omega |\lambda|^{2q} + \rho_q\Big(\frac{\lambda - \lambda_\tau^{k-1}}{\tau}\Big)\,{\rm d}x \\ &\text{subject to} \quad \lambda \in L^{2q}(\Omega;\mathbb{R}^{M+1}), \end{aligned}\right\} \tag{5.103a}$$

with $\mathcal{G}$ from (5.6).

2. The **minimization problem for** (y, ν) with given λ_τ^k:

$$\left.\begin{aligned} &\text{Minimize} \quad \mathfrak{G}(k\tau, y, \nu, \lambda_\tau^k) \\ &\text{subject to} \quad (y,\nu) \in W^{1,p}(\Omega;\mathbb{R}^d) \times \mathscr{G}^p_{\Gamma_{\rm D}}(\Omega;\mathbb{R}^{d\times d}) \\ &\qquad\qquad \text{such that } \nabla y = {\rm id} \bullet \nu \text{ a.e. on } \Omega. \end{aligned}\right\} \tag{5.103b}$$

with $\mathfrak{G}$ the mechanical part of $\mathcal{G}$ defined in (5.93),

3. The **enthalpy equation**: For all $\varphi \in W^{1,2}(\Omega)$

$$\begin{aligned} \int_\Omega \frac{w_\tau^k - w_\tau^{k-1}}{\tau}\varphi + \mathcal{K}(\lambda_\tau^k, w_\tau^k)\nabla w_\tau^k \cdot \nabla\varphi \,{\rm d}x + \int_\Gamma b_\tau^k \Theta(w_\tau^k)\varphi \,{\rm d}S = \int_\Gamma b_\tau^k \theta_{{\rm ext},\tau}^k \varphi \,{\rm d}S \\ + \int_\Omega \varrho\Big(\frac{\lambda_\tau^k - \lambda_\tau^{k-1}}{\tau}\Big)\varphi + \Theta(w_\tau^k)\vec{a}\cdot\frac{\lambda^k - \lambda^{k-1}}{\tau}\varphi \,{\rm d}x. \end{aligned} \tag{5.103c}$$

4. For $k = 0$ the **initial conditions** in the following sense

$$\nu_\tau^0 = \nu_0, \qquad \lambda_\tau^0 = \lambda_{0,\tau}, \qquad w_\tau^0 = w_{0,\tau} \quad \text{ on } \Omega. \tag{5.103d}$$

Where, in (5.103d), we denoted by $\lambda_{0,\tau} \in L^{2q}(\Omega;\mathbb{R}^{M+1})$ and $w_{0,\tau} \in L^2(\Omega)$, respectively, suitable approximation of the original initial conditions $\lambda_0 \in L^q(\Omega;\mathbb{R}^{M+1})$ and $w_0 \in L^1(\Omega)$ defined analogously to (5.41) and (5.42).

Again, as in (5.40a), we have added the regularization term $\tau|\lambda|^{2q}$ to minimization problem (5.103a) to assure enough integrability of the right-hand side of the discrete enthalpy equation 5.103c to prove existence of solutions to it. Again, this regularization term converges to 0 as $\tau \to 0$.

Remark 5.13 (On the choice of altering minimization in (5.103)). When comparing (5.103) to (5.40) on can observe that, while in (5.40) we obtain the discrete vector of volume fraction and the discrete microstructure from *one* minimization principle, in (5.103) we first obtain λ_τ^k *using* ν_τ^{k-1} in (5.103a) and only subsequently ν_τ^k through (5.103b).

The definition (5.103) is indeed *carefully devised* in order to assure that in the discrete flow-rule (5.111) (below) the term $\mathcal{Q}'_\varkappa(\bar\lambda_\tau - L\bullet\underline{\nu}_\tau)\cdot(v_\tau - \dot\lambda_\tau)$ will be present *instead of* the term $\mathcal{Q}'_\varkappa(\bar\lambda_\tau - L\bullet\bar\nu_\tau)\cdot(v_\tau - \dot\lambda_\tau)$ which we would get from a combined minimization principle. This will allow us to reformulate the discrete flow-rule (5.111) with the help of the discrete mechanic energy inequality (5.112), which is will be *crucial step* in the proof Theorem 5.15 below; recall that a similar reformulation was also used in the proof Theorem 5.12.

5.5.2 Existence of discrete solutions, a-priori estimates

Lemma 5.14. *Let (A1)-(A7) hold and let also $w_\tau^0 \geq 0$. Then there exists a discrete weak solution of (5.17a) in the sense of (5.103)such that $w_\tau^k \geq 0$ for all $k = 1 \dots T/\tau$.*

Moreover, the piecewise constant/affine interpolants of these discrete weak solutions defined as

$$\begin{aligned}\big[\bar y_\tau, \bar\nu_\tau, \bar\lambda_\tau, \bar w_\tau\big](t) &= \big(y_\tau^k, \nu_\tau^k, \lambda_\tau^k, w_\tau^k\big),\\ \big[\lambda_\tau, w_\tau\big](t) &= \frac{t-(k-1)\tau}{\tau}\big(\lambda_\tau^k, w_\tau^k\big) + \frac{k\tau - t}{\tau}\big(\lambda_\tau^{k-1}, w_\tau^{k-1}\big),\end{aligned}$$

for $(k-1)\tau < t \leq k\tau$ and $k = 1, ..., T/\tau$, satisfy the following bounds:

$$\sup_{t\in[0,T]} \int_\Omega |\cdot|^p \bullet \bar\nu_\tau \,\mathrm{d}x \leq C, \tag{5.104}$$

$$\big\|\dot{\bar\lambda}_\tau\big\|_{L^q(Q;\mathbb{R}^{M+1})} \leq C, \tag{5.105}$$

$$\big\|\bar\lambda_\tau\big\|_{L^\infty([0,T];L^{2q}(\Omega;\mathbb{R}^{M+1}))} \leq C\tau^{-1/2q}, \tag{5.106}$$

$$\big\|\bar w_\tau\big\|_{L^\infty([0,T];L^1(\Omega))} \leq C, \tag{5.107}$$

$$\big\|\nabla \bar w_\tau\big\|_{L^r(Q;\mathbb{R}^d)} \leq C_r \qquad \text{with any } \ 1 \leq r < \frac{d+2}{d+1}, \tag{5.108}$$

$$\big\|\dot{\bar w}_\tau\big\|_{\mathcal{M}([0,T];W^{1,\infty}(\Omega)^*)} \leq C. \tag{5.109}$$

Let us point out, that the *generic constant* C in (5.104)-(5.109) does *not* depend on τ. Also, within the proof, we shall use the notion of "retarded" enthalpy and microstructure piecewise constant interpolant $\underline{w}_\tau$, $\underline{\nu}_\tau$ defined by

$$[\underline{w}_\tau(t), \underline{\nu}_\tau(t)] := [w_\tau^{k-1}, \nu_\tau^{k-1}] \qquad \text{for } \ (k-1)\tau < t \leq k\tau, \ \ k = 1, ..., T/\tau. \tag{5.110}$$

Proof. Similarly as (5.40), we devised also (5.103) in such a way that (5.103a) is decoupled from (5.103b) as well as (5.103c). Therefore, we first show existence of solutions to (5.103a). To do so, we proceed by the *direct method* (cf. e.g. (Dacorogna, 1989) or the beginning of Section 2.2) relying on *convexity* of $\mathcal{G}$ in λ and *convexity* of the dissipation potential as well as in the regularization term $\tau\|\lambda|^{2q}$.

For (5.103b) we proceed by the direct method, too. Indeed, any minimizing sequence $\{[y_\tau^k]_j, [\nu_\tau^k]_j\}_{j\in\mathbb{N}}$ of the cost functional in (5.103b) satisfies that $\int_\Omega |\cdot|^p \bullet [\nu_\tau^k]_j \,\mathrm{d}x \leq C$ and hence converges $[\nu_\tau^k]_j$ weakly* in $L^\infty_{\mathrm{w}}(\Omega; \mathcal{M}(\mathbb{R}^{d\times d}))$ to some ν_τ^k and (having the constrain $\nabla[y_\tau^k]_j = \mathrm{id} \bullet [\nu_\tau^k]_j$ a.e. on Ω in mind) $[y_\tau^k]_j$ converges to some y_τ^k weakly in $W^{1,p}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{M+1})$; the limits satisfy that $\nabla y_\tau^k = \mathrm{id} \bullet \nu_\tau^k$ a.e. on Ω. Moreover, again thanks to the bound $\int_\Omega |\cdot|^p \bullet [\nu_\tau^k]_j \,\mathrm{d}x \leq C$ ν_τ^k is also a gradient Young measure owing to Theorem 2.14. Exploiting the weak lower semi-continuity of our cost functional (proved similarly as Lemma 2.11) gives that ν_τ^k is indeed the minimizer of (5.103b).

The existence of solutions to (5.103c) and the fact that $w_\tau^k \geq 0$ is proved analogously to *Step 1* in the proof Proposition 5.9.

As to the a-priori estimates (5.104)-(5.109), notice that the sub-differential of the cost function in (5.103a) with respect to λ has to be zero at λ_τ^k at each time level l. Summing these conditions up to some k and denoting $t_k = k\tau$ leads to

$$\begin{aligned}\int_0^{t_k}\!\!\int_\Omega \rho_q(\dot{\bar\lambda}_\tau)\,\mathrm{d}x\,\mathrm{d}t \leq \int_0^{t_k}\!\!\int_\Omega \Big(&\mathcal{Q}'_{\varkappa}(\bar\lambda_\tau - L\bullet\underline{\nu}_\tau)\cdot(v_\tau - \dot{\bar\lambda}_\tau)\\ &+ \big(\Theta(\underline{w}_\tau) - \theta_{\mathrm{tr}}\big)\vec a\cdot(v_\tau - \dot{\bar\lambda}_\tau) + 2q\tau|\bar\lambda_\tau|^{2q-2}\bar\lambda_\tau(v_\tau - \dot{\bar\lambda}_\tau) + \rho_q(v_\tau)\Big)\,\mathrm{d}x\,\mathrm{d}t,\end{aligned} \tag{5.111}$$

where v_τ is an arbitrary test function such that $v_\tau(\cdot,x)$ is piecewise constant on the intervals $(t_{j-1},t_j]$ and $v_\tau(t_j,\cdot)\in L^{2q}(\Omega;\mathbb{R}^{M+1})$ for every j.

Further, we deduce a mechanic energy inequality as in (5.63); i.e. we test (5.103b) by $\underline{\nu}_\tau$ as in (5.62)

$$\mathfrak{G}(t_k,\bar{\nu}_\tau(t_k),\bar{\lambda}_\tau(t_k))\le\mathfrak{G}(t_k,\underline{\nu}_\tau(t_k),\bar{\lambda}_\tau(t_k)),$$

rewrite the right-hand side using convexity of $\mathfrak{G}$ in λ

$$\begin{aligned}\mathfrak{G}(t_k,\underline{\nu}_\tau(t_k),\bar{\lambda}_\tau(t_k))&\le\mathfrak{G}(t_{k-1},\underline{\nu}_\tau(t_k),\bar{\lambda}_\tau(t_{k-1}))\\&\quad+\int_{t_{k-1}}^{t_k}\mathfrak{G}'_t(t,\underline{\nu}_\tau(t_k))+\int_\Omega\mathcal{Q}'_\varkappa(\bar{\lambda}_\tau(t)-L\bullet\underline{\nu}_\tau(t_k))\cdot\dot{\lambda}_\tau(t)\,\mathrm{d}x\,\mathrm{d}t\end{aligned}$$

and sum from $1\dots k$ to obtain

$$\begin{aligned}\mathfrak{G}(t_k,\bar{\nu}_\tau(t_k),\bar{\lambda}_\tau(t_k))&\le\mathfrak{G}(0,\bar{\nu}_\tau(0),\bar{\lambda}_\tau(0))\\&\quad+\int_0^{t_k}\mathfrak{G}'_t(t,\underline{\nu}_\tau(t_k))+\int_\Omega\mathcal{Q}'_\varkappa(\bar{\lambda}_\tau(t)-L\bullet\underline{\nu}_\tau(t_k))\cdot\dot{\lambda}_\tau(t)\,\mathrm{d}x\,\mathrm{d}t.\end{aligned}\tag{5.112}$$

Finally, summing the discrete version of the enthalpy equation (5.103c) from 1 to k leads to

$$\begin{aligned}&\int_0^{t_k}\Big(\int_\Omega\dot{w}_\tau\varphi+\mathcal{K}(\bar{\lambda}_\tau,\bar{w}_\tau)\nabla\bar{w}_\tau\cdot\nabla\varphi\,\mathrm{d}x+\int_\Gamma\bar{b}_\tau\Theta(\bar{w}_\tau)\varphi\,\mathrm{d}S\Big)\,\mathrm{d}t\\&\qquad=\int_0^{t_k}\Big(\int_\Omega(\varrho_q(\dot{\lambda}_\tau)+\Theta(\bar{w}_\tau)\vec{a}\cdot\dot{\lambda}_\tau)\varphi\,\mathrm{d}x+\int_\Gamma\bar{b}_\tau\bar{\theta}_{\mathrm{ext},\tau}\varphi\,\mathrm{d}S\Big)\,\mathrm{d}t,\end{aligned}\tag{5.113}$$

where φ is an arbitrary test function, such that $\varphi(\cdot,x)$ is piecewise constant on the intervals $(t_{j-1},t_j]$ and $\varphi(t_j,\cdot)\in W^{1,2}(\Omega)$ for every j.

In order to obtain (5.104)-(5.109) from (5.111), (5.112) and (5.113), we mimic the proof Lemma 5.10, i.e. we combine (5.112) with the result of the test of (5.111) by 0 and the result of the test of (5.113) by 1 to obtain (5.104)-(5.107) as in *Step 1* and *Step 2* of the proof Lemma 5.10. Subsequently, we test (5.113) by $1-\frac{1}{(1+\bar{w}_\tau)^a}$ to obtain (5.108); while (5.109) is got from (5.113) itself. □

5.5.3 Convergence towards the continuous case

Theorem 5.15 (Convergence for $\tau\to0$)**.** *Let the assumptions (A1)-(A7) hold. Then there exist* $(y,\nu,\lambda,w)\in B([0,T];W^{1,p}_{\Gamma_\mathrm{D}}(\Omega;\mathbb{R}^d))\times(\mathscr{G}^p_{\Gamma_\mathrm{D}}(\Omega;\mathbb{R}^{d\times d}))^{[0,T]}\times$
$W^{1,q}([0,T];L^q(\Omega;\mathbb{R}^{M+1}))\times L^r([0,T];W^{1,r}(\Omega))$ *and a sequence* $\tau\to0$ *such that*

$$\bar{\lambda}_\tau\overset{*}{\rightharpoonup}\lambda\qquad\text{in } L^\infty([0,T];L^q(\Omega,\mathbb{R}^{M+1}))\tag{5.114}$$

$$\bar{\lambda}_\tau(t)\rightharpoonup\lambda(t)\qquad\forall t\in[0,T]\ \text{ in } L^q(\Omega;\mathbb{R}^{M+1}),\tag{5.115}$$

$$\dot{\lambda}_\tau\to\dot{\lambda}\qquad\text{in } L^q(Q;\mathbb{R}^{M+1}),\tag{5.116}$$

$$\bar{w}_\tau\rightharpoonup w\qquad L^r([0,T];W^{1,r}(\Omega)),\ r<\tfrac{d+2}{d+1}\ \text{ and }\ \bar{w}_\tau\to w\ \text{ in } L^1(Q),\tag{5.117}$$

with (λ_τ,w_τ) *the piecewise affine interpolants and* $(\bar{\lambda}_\tau,\bar{w}_\tau)$ *the piecewise constant interpolants defined in Lemma 5.14.*
Moreover, for each $t\in[0,T]$ *there exists a subsequence* $\tau_{k(t)}$ *such that*

$$\bar{y}_{\tau_{k(t)}}(t)\overset{*}{\rightharpoonup}y(t)\quad\text{in } W^{1,p}(\Omega;\mathbb{R}^d)\qquad\bar{\nu}_{\tau_{k(t)}}(t)\overset{*}{\rightharpoonup}\nu(t)\quad\text{in } L^\infty_\mathrm{w}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d})),\tag{5.118}$$

such that $\nabla y(x)=\mathrm{id}\bullet\nu_x$ *for a.a.* $x\in\Omega$*; note that again* $(\bar{y}_\tau,\bar{\nu}_\tau)$ *were defined in Lemma 5.14.*

At least one cluster point (y,ν,λ,w) *obtained in this way is then a weak solution of (5.17) in accord with Definition 5.4.*

Proof. As already mentioned, the proof combines arguments from *Steps 4-7* from the proof Proposition 5.14 and of Theorem 5.12. For clarity, let us divide it into several steps:

Step 1: Selection of subsequences, reformulating and limiting the flow-rule
Exploiting the a-priori estimates (5.105)-(5.109) we choose, analogously to *Step 3* of the proof Proposition 5.9, a subsequence of τ's (not relabeled) such that (5.114), (5.115), (5.117) and

$$\dot{\lambda}_\tau \overset{*}{\rightharpoonup} \dot{\lambda} \quad \text{in } L^q(Q;\mathbb{R}^{M+1}), \tag{5.119}$$

hold. Also, as in *Step 1* of Theorem 5.12, $\Theta(\bar{w}_\tau) \to \Theta(w)$ in $L^{q'}(Q)$ and, due to (5.109), $\Theta(\underline{w}_\tau) \to \Theta(w)$ in $L^{q'}(Q)$, too.

Following *Step 1* of the proof Theorem 5.12, we reformulate (5.111) using (5.112) into a yet weaker form to (partially) cope with the problem of measurability of $\int_\Omega \mathcal{Q}'_\varkappa(\lambda(t)-L\bullet\nu(t))\cdot(v(t)-\dot{\lambda})\,\mathrm{d}x$.

To do so, let us first abbreviate

$$\begin{aligned}\mathfrak{G}_\tau(T) &:= \mathfrak{G}(T,\bar{y}_\tau(T),(T)\bar{\nu}_\tau(T),\bar{\lambda}_\tau(T)),\\ \mathfrak{G}_\tau(0) &:= \mathfrak{G}(0,\bar{y}_\tau(0),\bar{\nu}_\tau(0),\bar{\lambda}_\tau(0));\end{aligned}$$

with this notation, plugging (5.112) into (5.111)[27] yields the following *reformulated flow rule*:

$$\begin{aligned}\int_\Omega |\bar{\lambda}_\tau(T)|^{2q}\,\mathrm{d}x+\int_Q \rho_q(\dot{\lambda}_\tau)\,\mathrm{d}x\,\mathrm{d}t \le \int_\Omega |\lambda_{0,\tau}|^{2q}\,\mathrm{d}x+\int_Q \mathcal{Q}'_\varkappa(\bar{\lambda}_\tau-L\bullet\underline{\nu}_\tau)\cdot v_\tau\,\mathrm{d}x\,\mathrm{d}t+\int_0^T \mathfrak{G}'_t(t,\underline{\nu}_\tau)\,\mathrm{d}t\\ +\int_Q \Big(\rho_q(v_\tau)+(\Theta(\underline{w}_\tau)-\theta_{\mathrm{tr}})\vec{a}\cdot(v_\tau-\dot{\lambda}_\tau)+2q\tau|\lambda_\tau|^{2q-2}\bar{\lambda}_\tau\cdot v_\tau\Big)\,\mathrm{d}x\,\mathrm{d}t+\mathfrak{G}_\tau(0)-\mathfrak{G}_\tau(T).\end{aligned} \tag{5.120}$$

we further, relying on the linearity of $\mathcal{Q}'_\varkappa$ (see (5.2)), rewrite (5.120) as

$$\begin{aligned}\int_\Omega |\bar{\lambda}_\tau(T)|^{2q}\,\mathrm{d}x+\int_Q \rho_q(\dot{\lambda}_\tau)\,\mathrm{d}x\,\mathrm{d}t \le \int_\Omega |\lambda_{0,\tau}|^{2q}\,\mathrm{d}x+\int_Q \mathcal{Q}'_\varkappa(\bar{\lambda}_\tau-L\bullet\bar{\nu}_\tau)\cdot v_\tau\,\mathrm{d}x\,\mathrm{d}t+\int_0^T \mathfrak{G}'_t(t,\bar{\nu}_\tau)\,\mathrm{d}t\\ +\int_Q \Big(\rho_q(v_\tau)+(\Theta(\underline{w}_\tau)-\theta_{\mathrm{tr}})\vec{a}\cdot(v_\tau-\dot{\lambda}_\tau)+2q\tau|\lambda_\tau|^{2q-2}\bar{\lambda}_\tau\cdot v_\tau\Big)\,\mathrm{d}x\,\mathrm{d}t\\ \int_Q \mathcal{Q}'_\varkappa(L\bullet\bar{\nu}_\tau-L\bullet\underline{\nu}_\tau)\cdot v_\tau+\int_0^T \mathfrak{G}'_t(t,\underline{\nu}_\tau)-\mathfrak{G}'_t(t,\bar{\nu}_\tau)\,\mathrm{d}t\mathfrak{G}_\tau(0)-\mathfrak{G}_\tau(T).\end{aligned} \tag{5.121}$$

just to make the limit passage below easier.

Let us now pass to the limit $\tau\to 0$ in (5.121). As in *Step 1* of the proof Theorem 5.12, we choose a test function $v\in\mathcal{V}$, where $\mathcal{V}$ is a countable dense subset of $L^q(Q;\mathbb{R}^{M+1})$, considered *fixed* at the moment. Further consider its piecewise constant approximations v_τ such that $v_\tau\to v$ strongly on $L^q(Q;\mathbb{R}^{d+1})$ such that $\|v_\tau\|_{L^{2q}(Q;\mathbb{R}^{d+1})}\le C\tau^{-1/(2q+1)}$ and moreover $v_\tau(t)\to v(t)$ strongly in $L^q(\Omega;\mathbb{R}^{d+1})$ for a.a. $t\in[0,T]$.

Using weak lower semi-continuity properties (see also *Step 4* in the proof Proposition 5.9), we get that $\int_Q \rho_q(\dot{\lambda})\,\mathrm{d}x\,\mathrm{d}t \le \liminf_{\tau\to 0}\int_\Omega \tau|\bar{\lambda}_\tau(T)|^{2q}\,\mathrm{d}x+\int_Q \rho_q(\dot{\lambda}_\tau)\,\mathrm{d}x\,\mathrm{d}t$.

On the right-hand side of (5.121), we use, as in *Step 4* in the proof Proposition 5.9 that $\Theta(\underline{w}_\tau)\to\Theta(w)$ in $L^{q'}(Q)$ to pass to the limit in $\int_Q(\Theta(\underline{w}_\tau)-\theta_{\mathrm{tr}})\vec{a}\cdot(v_\tau-\dot{\lambda}_\tau)\,\mathrm{d}x\,\mathrm{d}t$. Moreover, due to the controlled blow-up of $\lambda_{0,\tau}$ the term $\tau\int_\Omega|\lambda_{0,\tau}|^{2q}\,\mathrm{d}x$ converges to 0. Also the term $2q\tau|\bar{\lambda}_\tau|^{2q-2}\bar{\lambda}_\tau v_\tau$ can be pushed to zero thanks to (5.106) and the

[27] We use both integrated to T; i.e. $k=N$ in (5.112) and (5.111).

blow-up for v_τ specified above that allow us to estimate $\int_Q 2q\tau|\bar\lambda_\tau|^{2q-2}\bar\lambda_\tau v_\tau|\,\mathrm{d}x\,\mathrm{d}t \le 2q\tau\|\bar\lambda_\tau\|^{2q-1}_{L^{2q}(Q;\mathbb{R}^{d+1})}\|v_\tau\|_{L^{2q}(Q;\mathbb{R}^{d+1})} \le C\tau^{\frac{1}{4q^2+2q}}$. Eventually, since $\mathfrak{G}_\tau(0)$ and $\mathfrak{G}_\tau(T)$ are bounded sequences of numbers, we assume that $\lim_{\tau\to0}\mathfrak{G}_\tau(0)$ and $\lim_{\tau\to0}\mathfrak{G}_\tau(T)$ exist – if they did not, we could always find a sub-sequence of τ such that they existed.

Next let us show that the term $\int_0^T \varkappa(L\bullet\bar\nu_\tau - L\bullet\underline{\nu}_\tau)\cdot(v_\tau)\rangle\!\rangle$ converges to 0 if $\tau\to0$. To this point it suffices to prove that $(L\bullet\bar\nu_\tau - L\bullet\underline{\nu}_\tau)$ converges weakly to 0 in $L^2([0,T];L^2(\Omega;\mathbb{R}^{M+1}))$. To see this, take the test functions $\xi_{[k\tau,l\tau]}g(x)$, $k,l>0$ (ξ_A being here the characteristic function of the set A, i.e. ξ is 1 in A and 0 elsewhere, and $g\in L^2(\Omega;\mathbb{R}^{M+1})$ arbitrary) which are dense in $L^2(Q;\mathbb{R}^{M+1})$ and compute (by substitution)

$$\begin{aligned}
&\Big|\int_Q (L\bullet\bar\nu_\tau - L\bullet\underline{\nu}_\tau)\xi_{[k\tau,l\tau]}g\,\mathrm{d}x\,\mathrm{d}t\Big| \\
&\quad= \Big|\int_{k\tau}^{l\tau}\int_\Omega (L\bullet\bar\nu_\tau(t))g\,\mathrm{d}x\,\mathrm{d}t - \int_{(k-1)\tau}^{(l-1)\tau}\int_\Omega (L\bullet\bar\nu_\tau(t))g\,\mathrm{d}x\,\mathrm{d}t\Big| \\
&\quad= \Big|\int_{k\tau}^{l\tau}\int_\Omega (L\bullet\bar\nu_\tau(t))g\,\mathrm{d}x\,\mathrm{d}t - \int_{k\tau}^{l\tau}\big(\int_\Omega L\bullet\bar\nu_\tau(t))g\,\mathrm{d}x\,\mathrm{d}t \\
&\qquad\qquad - \int_{(k-1)\tau}^{k\tau}\int_\Omega (L\bullet\bar\nu_\tau(t))g\,\mathrm{d}x\,\mathrm{d}t + \int_{(l-1)\tau}^{l\tau}\int_\Omega (L\bullet\bar\nu_\tau(t))g\,\mathrm{d}x\,\mathrm{d}t\Big| \\
&\quad= \tau\Big|\int_\Omega (L\bullet\bar\nu_\tau(k\tau) + L\bullet\bar\nu_\tau(l\tau))g\,\mathrm{d}x\Big| \le \tau|\Omega| \to 0.
\end{aligned} \tag{5.122}$$

Similarly, the term $\int_0^T \mathfrak{G}_t'(t,\underline{\nu}_\tau(t))\,\mathrm{d}t - \mathfrak{G}_t'(t,\bar\nu_\tau(t))\,\mathrm{d}t = \int_0^T\big(\int_\Omega f(\underline{y}_\tau-\bar y_\tau)\,\mathrm{d}x + \int_{\Gamma_{\mathrm{N}}}(g(\underline{y}_\tau-\bar y_\tau))\,\mathrm{d}S\big)\,\mathrm{d}t$ converges to 0. Indeed, one only needs to show that $(\underline{y}_\tau-\bar y_\tau)\to0$ weakly in $L^p([0,T];W^{1,p}(\Omega;\mathbb{R}^d))$. However, thanks to the zero Dirichlet boundary condition on Γ_{D}, it is enough to show that $(\nabla\underline{y}_\tau - \nabla\bar y_\tau) = (\mathrm{id}\bullet\underline{\nu}_\tau - \mathrm{id}\bullet\bar\nu_\tau)$ converges weakly to 0 in $L^p(Q;\mathbb{R}^{d\times d})$; for this we proceed as in (5.122) and realize that $\big|\int_\Omega(\mathrm{id}\bullet\bar\nu_\tau(k\tau) + \mathrm{id}\bullet\bar\nu_\tau(l\tau))g\,\mathrm{d}x\big| \le C$ (where C is independent of k,l and τ) thanks to (5.104).

Therefore, similarly as in *Step 1* of the proof Theorem 5.12, the most problematic terms on the right-hand-side of the flow rule are $\mathcal{Q}'_\varkappa(\lambda - L\bullet\bar\nu_\tau)\cdot v_\tau$ and $[\mathfrak{G}]'_t(t,\bar\nu_\tau(t))$; we circumpass the problems by exploiting the same procedure as in as in *Step 1* of the proof Theorem 5.12 inspired by (Dal Maso et al., 2005; Francfort and Mielke, 2006). Hence, we define $\bar{\mathcal{L}}^v(t)$ *dependent on the choice of the test function* v as well as the function $\bar{\mathcal{F}}(t)$ through

$$\bar{\mathcal{L}}^v(t) = \limsup_{\tau\to0}\int_\Omega \mathcal{Q}'_\varkappa(\bar\lambda_\tau(t) - L\bullet\bar\nu_\tau(t))\cdot v(t)\,\mathrm{d}x, \quad \bar{\mathcal{F}}(t) = \limsup_{\tau\to0}[\mathfrak{G}]'_t(t,\bar\nu_\tau(t)). \tag{5.123}$$

Thanks to Fatou's lemma[28], $\bar{\mathcal{L}}^v(t)$, $\bar{\mathcal{F}}(t)$ are measurable and

$$\begin{aligned}
&\limsup_{\tau\to0}\int_0^T\int_\Omega \mathcal{Q}'_\varkappa(\bar\lambda_\tau - L\bullet\bar\nu_\tau)\cdot v_\tau\,\mathrm{d}x\,\mathrm{d}t \\
&\quad\le \limsup_{\tau\to0}\int_Q \mathcal{Q}'_\varkappa(\bar\lambda_\tau - L\bullet\bar\nu_\tau)\cdot v\,\mathrm{d}x + \limsup_{\tau\to0}\int_Q \mathcal{Q}'_\varkappa(\bar\lambda_\tau - L\bullet\bar\nu_\tau)\cdot(v_\tau - v) \le \int_0^T \bar{\mathcal{L}}^v\,\mathrm{d}t, \\
&\limsup_{\tau\to0}\int_0^T [\mathfrak{G}]'_t(t,\bar\nu_\tau(t)) \le \int_0^T \bar{\mathcal{F}}\,\mathrm{d}t,
\end{aligned}$$

where we used that $\mathcal{Q}'_\varkappa(\bar\lambda_\tau - L\bullet\bar\nu_\tau)$ is uniformly bounded in $L^\infty([0,T],L^2(\Omega,\mathbb{R}^{M+1}))$ (cf. (5.104), (5.105)) and $v_\tau\to v$ strongly in $L^q(Q;\mathbb{R}^{M+1})$. Hence we may apply $\liminf_{\tau\to0}$

[28] More information on the applicability of Fatou's lemma can be found in the text below (5.88).

to both sides of (5.121) and use the for the right-hand-side the "lim inf $\leq$ lim sup" inequality to get

$$\int_0^T\int_\Omega \rho_q(\dot\lambda) \leq \int_0^T \bar{\mathcal{L}}^v+\bar{\mathcal{F}}\,\mathrm{d}t+\int_0^T\int_\Omega(\Theta(w)-\theta_{\mathrm{tr}})\vec{a}\cdot(v-\dot\lambda)+\delta_S^*(v)+\frac{\alpha}{q}|v|^q\,\mathrm{d}x\,\mathrm{d}t + \lim_{\tau\to 0}\mathfrak{G}_\tau(0)-\lim_{\tau\to 0}\mathfrak{G}_\tau(T), \tag{5.124}$$

Fix some time $t\in[0,T]$. Then for any $v\in\mathcal{V}$ we may find a time-dependent subsequence of τ's denoted $\tau_{k_{(t,v)}}$, such that[29]

$$\bar{\mathcal{L}}^v(t)=\lim_{\tau_{k_{(t,v)}}\to 0}\int_\Omega \mathcal{Q}'_\varkappa(\bar\lambda_{\tau_{k_{(t,v)}}}-L\bullet\bar\nu_{\tau_{k_{(t,v)}}})\cdot\,\mathrm{d}x \tag{5.125}$$

$$\mathcal{F}(t)=\lim_{\tau_{k_{(t,v)}}\to 0}[\mathfrak{G}]'_t(t,\bar\nu_{\tau_{k_{(t,v)}}}(t))=\lim_{\tau_{k_{(t,v)}}\to 0}\int_\Omega \dot f(t)\bar y_{\tau_{k_{(t,v)}}}(t)\,\mathrm{d}x+\int_{\Gamma_{\mathrm{N}}}\dot g(t)\bar y_{\tau_{k_{(t,v)}}}(t)\,\mathrm{d}S. \tag{5.126}$$

By diagonal selection find a further subsequence labeled $\tau_{k(t)}$, such that (5.125) - (5.126) hold *even for all* $v\in\mathcal{V}$.

Using the second estimate in (5.104) we may again select a subsequence of $\tau_{k(t)}$'s (not relabeled) such that $\nu_{\tau_{k(t)}}$ converges weakly* to $\nu(t)$ in $L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d}))$, note that (5.104) also guarantees that the limit $\nu(t)\in\mathscr{G}^p_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^{d\times d})$ and, combined with (A3), that $L\bullet\bar\nu_{\tau_{k(t)}}(t)\to L\bullet\nu(t)$ weakly in $L^2(\Omega;\mathbb{R}^{M+1})$.

Therefore (5.125) and (5.126) yield

$$\bar{\mathcal{L}}^v(t)=\int_\Omega \mathcal{Q}'_\varkappa(\lambda(t)-L\bullet\nu(t))\cdot v(t),$$
$$\mathcal{F}(t)=\int_\Omega f(t)\cdot y(t)\,\mathrm{d}x+\int_{\Gamma_{\mathrm{N}}} g(t)\cdot y(t)\,\mathrm{d}S,$$

for all $v\in\mathcal{V}$.

This allows us to rewrite (5.124) for all $v\in\mathcal{V}$ as

$$\int_0^T\int_\Omega\rho_q(\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t\leq\int_0^T\int_\Omega\mathcal{Q}'_\varkappa(\lambda-L\bullet\nu)\cdot v+\int_\Omega f\cdot y\,\mathrm{d}x+\int_{\Gamma_{\mathrm{N}}}g\cdot y\,\mathrm{d}S\,\mathrm{d}t + \int_Q(\Theta(w)-\theta_{\mathrm{tr}})\vec{a}\cdot(v-\dot\lambda)+\rho_q(v)+\lim_{\tau\to0}\mathfrak{G}_\tau(0)-\lim_{\tau\to0}\mathfrak{G}_\tau(T)\,\mathrm{d}x\,\mathrm{d}t. \tag{5.127}$$

This can be generalized to all $\tilde v\in L^q(Q;\mathbb{R}^{M+1})$ by a density argument as in *Step 1* of the proof Theorem 5.12.

Step 2: Limiting the minimization principle, energy inequality, back to original flow-rule

Let $t\in[0,T]$ *be still fixed.* Let us, moreover, denote $t_{\tau_{k(t)}}=l\cdot\tau_{k(t)}$, where $l=\min_{s\in\mathbb{N}}\{t\leq s T/\tau_{k(t)}\}$. Then due to the coercivity of the stored energy (cf. (A1)) and a lower semi-continuity property analogousto Lemma 2.11 we may write[30]

$$\mathfrak{G}(t,y(t),\nu(t),\lambda(t))\leq\liminf_{\tau_{k(t)}\to0}\mathfrak{G}(t_{\tau_{k(t)}},\bar y_{\tau_{k(t)}}(t).\bar\nu_{\tau_{k(t)}}(t),\bar\lambda_{\tau_{k(t)}}(t)) \leq\liminf_{\tau_{k(t)}\to0}\mathfrak{G}(t_{\tau_{k(t)}},\tilde y,\tilde\nu,\bar\lambda_{\tau_{k(t)}}(t))=\mathfrak{G}(t,\tilde y,\tilde\nu,\lambda(t)). \tag{5.128}$$

for any pair $(\tilde y,\tilde\nu)\in W^{1,p}_{\Gamma_{\mathrm{D}}}(\Omega;\mathbb{R}^d)\times\mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^{d\times d})$ such that $\nabla\tilde y=\mathrm{id}\bullet\nu$ a.e. on Ω, which gives the desired minimization principle (5.22).

[29] This is analogousto the procedure of (5.90)-(5.91).

[30] For more details, we refer also to *Step 2* of the proof Theorem 5.12.

Note that, we also get that $\mathfrak{G}(t,\nu(t),\lambda(t)) = \lim_{\tau_{k(t)}\to 0}\mathfrak{G}(t,\bar{\nu}_{\tau_{k(t)}}(t),\bar{\lambda}_{\tau_{k(t)}}(t))$ by this procedure; in particular, this means that

$$\left.\begin{aligned}\mathfrak{G}(0) \equiv \mathfrak{G}(0,\nu(0),\lambda(0)) = \lim_{\tau\to 0}\mathfrak{G}_\tau(0),\\ \mathfrak{G}(T) \equiv \mathfrak{G}(T,\nu(T),\lambda(T)) = \lim_{\tau\to 0}\mathfrak{G}_\tau(T).\end{aligned}\right\} \tag{5.129}$$

Note that, once we obtained (5.22), we also got (5.97) by *Step 3* of the proof Theorem 5.12, which, in turn, yields (5.23) from (5.127).

Step 3: Strong convergence of $\dot{\lambda}$ and convergence in the enthalpy equation

To prove (5.116), we combine the arguments from *Step 5* of the proof Proposition (5.9) and *Step 3* of the proof Theorem 5.12. Hence, we test the discrete flow rule (cf. 5.121, *rewritten using convexity of* $|\cdot|^q$) by $\dot{\lambda}_{\mathrm{S},\tau,k}$ with $\dot{\lambda}_{\mathrm{S},\tau,k}$ being a piecewise constant approximation of the function $\dot{\lambda}_k$ such that $\dot{\lambda}_{\mathrm{S},\tau,k}\to\dot{\lambda}_k$ strongly in $L^q(Q;\mathbb{R}^{M+1})$ and moreover $\|\dot{\lambda}_{\mathrm{S},\tau,k}\|_{L^{2q}(Q;\mathbb{R}^{M+1})}\le C\tau^{-1/(2q+1)}$. $\dot{\lambda}_k$, on the other hand, is a function in $\mathcal{V}$ such that $\dot{\lambda}_k\to\dot{\lambda}$ in $L^q(Q;\mathbb{R}^{M+1})$ when $k\to\infty$.[31]; the outlined test gives

$$\begin{aligned}&\int_\Omega|\bar{\lambda}_\tau(T)|^{2q}\,\mathrm{d}x+\int_Q\delta_S^*(\dot{\lambda}_\tau)\,\mathrm{d}x\,\mathrm{d}t\le\mathfrak{G}_\tau(0)-\mathfrak{G}(T)+\int_\Omega|\bar{\lambda}_{0,\tau}|^{2q}\,\mathrm{d}x+\int_Q\delta_S^*(\dot{\lambda}_{\mathrm{S},\tau,k})\,\mathrm{d}x\,\mathrm{d}t\\
&\quad+\int_Q\alpha|\dot{\lambda}_\tau|^{q-2}\dot{\lambda}_\tau\cdot(\dot{\lambda}_{\mathrm{S},\tau,k}-\dot{\lambda}_\tau)+(\Theta(\underline{w}_\tau)-\theta_{\mathrm{tr}})\vec{a}\cdot(\dot{\lambda}_{\mathrm{S},\tau,k}-\dot{\lambda}_\tau)+2q\tau|\bar{\lambda}_\tau|^{2q-2}\bar{\lambda}_\tau\cdot\dot{\lambda}_{\mathrm{S},\tau,k}\,\mathrm{d}x\,\mathrm{d}t\\
&\quad+\int_Q\mathcal{Q}'_\varkappa(\bar{\lambda}_\tau-L\bullet\bar{\nu}_\tau)\cdot\dot{\lambda}_{\mathrm{S},\tau,k}+\int_0^T\mathfrak{G}'_t(t,\bar{y}_\tau(t))\,\mathrm{d}t\\
&\quad+\int_Q\mathcal{Q}'_\varkappa(L\bullet\bar{\nu}_\tau-L\bullet\underline{\nu}_\tau)\cdot\dot{\lambda}_{\mathrm{S},\tau,k}\,\mathrm{d}x\,\mathrm{d}t+\int_0^T\big(\mathfrak{G}'_t(t,\underline{y}_\tau(t))-\mathfrak{G}'_t(t,\bar{y}_\tau(t))\big)\,\mathrm{d}t\end{aligned}\tag{5.130}$$

Symmetrically test (5.127) (the reformulated limited flow-rule; here *again rewritten using the convexity of* $|\cdot|^q$), with limits of the mechanic part of the Gibbs free energy in the initial and final time identified by means of (5.129), by $\dot{\lambda}_\tau$ to get

$$\begin{aligned}&\int_Q\delta_S^*(\dot{\lambda})\,\mathrm{d}x\,\mathrm{d}t\le\mathfrak{G}(0)-\mathfrak{G}(T)+\int_Q\delta_S^*(\dot{\lambda}_\tau)+\alpha|\dot{\lambda}|^{q-2}\dot{\lambda}(\dot{\lambda}_\tau-\dot{\lambda})\,\mathrm{d}x\,\mathrm{d}t\\
&\qquad\int_Q\mathcal{Q}'_\varkappa(\lambda-L\bullet\nu)\cdot\dot{\lambda}_\tau+(\Theta(w)-\theta_{\mathrm{tr}})\vec{a}\cdot(\dot{\lambda}_\tau-\dot{\lambda})\,\mathrm{d}x\,\mathrm{d}t+\int_0^T\mathfrak{G}'_t(t,y)\,\mathrm{d}t\end{aligned}\tag{5.131}$$

Add (5.130) and (5.131) and apply $\limsup_{\tau\to 0}$ to get

[31] Note that we need to test the discrete flow-rule by a piecewise constant function and hence cannot use directly $\dot{\lambda}$. However, we neither can use directly the approximation of $\dot{\lambda}$ since we will need to exploit (5.123) which holds only for functions in a countable dense subset of $L^q(\Omega;\mathbb{R}^{M+1})$ in which $\dot{\lambda}$ does not need to lie. Hence we first approximate $\dot{\lambda}$ by functions from this countable subset and subsequently find piecewise constant approximations of these functions.

$$
\begin{aligned}
&\alpha \lim_{\tau\to 0}\Big(\|\dot\lambda_\tau\|^{q-1}_{L^q(Q;\mathbb{R}^{M+1})}-\|\dot\lambda\|^{q-1}_{L^q(Q;\mathbb{R}^{M+1})}\Big)\Big(\|\dot\lambda_\tau\|_{L^q(Q;\mathbb{R}^{M+1})}-\|\dot\lambda\|_{L^q(Q;\mathbb{R}^{M+1})}\Big)\\
&\quad\le \lim_{\tau\to 0}\alpha\int_Q\Big(|\dot\lambda_\tau|^{q-2}\dot\lambda_\tau-|\dot\lambda|^{q-2}\dot\lambda\Big)\cdot(\dot\lambda_\tau-\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t\\
&\quad\le \lim_{k\to\infty}\limsup_{\tau\to 0}\Bigg(\mathfrak{G}(0)-\mathfrak{G}(T)+\underbrace{\mathfrak{G}_\tau(0)-\mathfrak{G}_\tau(T)}_{\text{(I)}}+\int_0^T\underbrace{\mathfrak{G}'_t(t,\bar y_\tau)}_{\text{(II)}}+\mathfrak{G}'_t(t,y)\,\mathrm{d}t\\
&\quad+\int_Q\underbrace{\alpha|\dot\lambda_\tau|^{q-2}\dot\lambda_\tau(\dot\lambda_{\mathrm{S},\tau,k}-\dot\lambda)+\delta_S^*(\dot\lambda_{\mathrm{S},\tau,k})-\delta_S^*(\dot\lambda)}_{\text{(III)}}\,\mathrm{d}x\,\mathrm{d}t\\
&\quad+\int_Q\underbrace{\mathcal{Q}'_\varkappa(\bar\lambda_\tau-L\bullet\bar\nu_\tau)\cdot\dot\lambda_{\mathrm{S},\tau,k}}_{\text{(IV)}}+\underbrace{\mathcal{Q}'_\varkappa(L\bullet\bar\nu_\tau-L\bullet\underline{\nu}_\tau)\cdot\dot\lambda_{\mathrm{S},\tau,k}}_{\text{(V)}}+\underbrace{\varkappa\langle\!\langle\lambda-L\bullet\nu,\dot\lambda_\tau\rangle\!\rangle}_{\text{(VI)}}\,\mathrm{d}x\,\mathrm{d}t\\
&\quad+\int_0^T\int_\Omega\underbrace{(\Theta(\underline{w}_\tau)-\theta_{\mathrm{tr}})\vec a\cdot(\dot\lambda_{\mathrm{S},\tau,k}-\dot\lambda_\tau)+(\Theta(w)-\theta_{\mathrm{tr}})\vec a\cdot(\dot\lambda_\tau-\dot\lambda)}_{\text{(VII)}}\,\mathrm{d}x+\underbrace{(\mathfrak{G}'_t(t,{}_\tau)-\mathfrak{G}'_t(t,\bar y_\tau))}_{\text{(VIII)}}\mathrm{d}t\Bigg)\\
&\quad\le\lim_{k\to\infty}\Bigg(C\|\dot\lambda_k-\dot\lambda\|_{L^Q(Q;\mathbb{R}^{M+1})}+\int_Q\delta_S^*(\dot\lambda_k)-\delta_S^*(\dot\lambda)+(\Theta(w)-\theta_{\mathrm{tr}})\vec a\cdot(\dot\lambda_k-\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t\\
&\quad+\int_Q\mathcal{Q}'_\varkappa(\lambda-L\bullet\nu)\cdot(\dot\lambda_k+\dot\lambda)+\int_0^T 2\mathfrak{G}'_t(t,\nu)\,\mathrm{d}t-2\mathfrak{G}(T)+2\mathfrak{G}(0)\Bigg)\\
&\quad\le 2\Big(\int_0^T\mathcal{Q}'_\varkappa(\lambda-L\bullet\nu)\cdot\dot\lambda+\mathfrak{G}'_t(t,y)\,\mathrm{d}t-\mathfrak{G}(T)+\mathfrak{G}(0)\Big)\le 0,
\end{aligned}
\tag{5.132}
$$

i.e. (5.116) after exploiting the uniform convexity of $L^q(Q;\mathbb{R}^{M+1})$.[32]

Note that we usedm in (5.132), (5.129) for Term (I), the procedure from *Step 1* for Term (II) and Term(IV), (5.122) and 5.119 for Term (V) and Term(VIII), and the strong convergence of $\bar w_\tau$ (cf. *Step 1*) for all other terms.

The limit passage in the discrete enthalpy equation (5.103c) is done by the same means as in *Step 4* of the proof Theorem 5.12 – in fact, it is even easier here since we do not have to cope with the dissipated heat due to pinning effects as when transiting from the microscopic case. □

[32] See also *Step 5* of the proof Proposition 5.9 for details.

Chapter 6

Refinements in the analysis of thermally coupled model in the convex case

After having analyzed, in Chapter 5, thermally coupled model for single crystalline SMAs (5.17), let us illustrate in this chapter how the analysis can be simplified in the *convex*case and, also, to which extent it can be refined; note that the convex case corresponds to the situation in which we would allow ν in (5.6) or (5.17a) to range not only over the set of L^p-gradient Young measures but over the set of *all* L^p Young measures.

While for mesoscopic models of SMAs in the large deformation setting the convex setting leads to severe *under-relaxation*, for some special loading type of so-called anti-plane shear (see e.g. (Roubíček, 2000) or (Rieger and Zimmer, 2005) where a similar model has been analyzed in the 1-D case) or, in the very special case, of considering fixed volume fraction and *small strain setting* it was be proved that the quasiconvex envelope of the Helmholtz free energy is actually convex (Govindjee et al., 2002; Kohn, 1991) – in those situations the results from this chapter represent a correct relaxation.

Also, practically the same system as obtained in (6.1) below[1] finds its application when describing the ferro/paramagnetic transition in micromagnetism; this was actually done in (Benešová, Kružík and Roubíček, 2012).

As announced, in this section, we illustrate that Theorem 5.15 can be slightly refined in the convex case; cf. Remark 6.6. Moreover, in the convex case, we can pass to the limit $\varkappa \to \infty$ in the penalized problem (albeit the obtain weak formulation is *very weak*) – this presents a justification for the introduction of a penalty causing only a small mismatch between λ and $L \bullet \nu$, i.e. the phase field and the vector of volume fractions calculated from the microstructure, in Section 5.1.1.

6.1 Strong and weak formulation in the convex case

Since the convex case is understood to have rather an illustrative character within this thesis, we make *the simplifying assumption* that the volume force f and the surface force g in (5.6) are equal to 0. Then the relaxed Gibbs free energy $\mathcal{G}^{\mathrm{C}}$ reads as

$$\mathcal{G}^{\mathrm{C}}(\nu,\lambda,\theta)=\int_\Omega \tilde{\psi}_0 \bullet \nu + \mathcal{Q}'_\varkappa(\lambda - L\bullet\nu) + \phi_0(\theta) + (\theta-\theta_{\mathrm{tr}})\vec{a}\cdot\lambda \,\mathrm{d}x;$$

the dissipation potential from (5.9) stays unchanged.

[1] The system (6.1) is analogous to (5.17) only the convexity has been exploited.

Let us therefore define the *convex equivalent* of (5.17) in strong form as[2]

$$\left.\begin{array}{ll}\text{minimize} & \mathcal{G}^{\mathrm{C}}(\nu,\lambda_\varkappa,\theta_\varkappa)\\ \text{subject to} & \nu\in\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d}) \text{ with } (\lambda_\varkappa,\theta_\varkappa) \text{ fixed},\end{array}\right\} \qquad \text{for } t\in[0,T], \tag{6.1a}$$

$$\partial\delta_S^*(\dot\lambda_\varkappa)+\alpha|\dot\lambda_\varkappa|^{q-2}\dot\lambda_\varkappa+\Theta(w_\varkappa)\vec a\ni\theta_{\mathrm{tr}}\vec a-\varkappa\mathfrak{Q}^*\mathfrak{Q}(\lambda_\varkappa-L\bullet\nu_\varkappa) \qquad \text{in } Q, \tag{6.1b}$$

$$\dot w_\varkappa-\mathrm{div}(\mathcal{K}(\lambda_\varkappa,w_\varkappa)\nabla w_\varkappa)=\delta_S^*(\dot\lambda_\varkappa)+\alpha|\dot\lambda_\varkappa|^q+\Theta(w_\varkappa)\vec a\cdot\dot\lambda_\varkappa \qquad \text{in } Q, \tag{6.1c}$$

$$\big(\mathcal{K}(\lambda_\varkappa,w_\varkappa)\nabla w_\varkappa\big)\cdot n+b\Theta(w_\varkappa)=b\theta_{\mathrm{ext}} \qquad \text{on } \Sigma; \tag{6.1d}$$

where, as already announced, the minimization in (6.1a) is performed over the *convex* set $\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d})$. Note that, within this chapter, we shall use the index "$\varkappa$" for solutions of thermally coupled system featuring the penalization term $\mathcal{Q}_\varkappa(\cdot)$ to emphasize their dependence of the choice of $\varkappa$ is this term. The motivation behind this is that, contrary to e.g. Chapter 5, we *do not consider* $\varkappa$ *fixed* throughout the chapter but shall pass here with $\varkappa\to\infty$ in Section 6.3.

Remark 6.1. Note that, since we neglected volume and surface forces, the *unrelaxed* Gibbs free energy would depend *only* on the matrix F such that $F=\nabla y$ (and not directly on y). The idea behind convex relaxation is then to "forget about the constraint that $F=\nabla y$, i.e. that it is the generalized gradient to some function in $L^p(\Omega;\mathbb{R}^d)$", and rather consider F as an arbitrary function in $L^p(\Omega;\mathbb{R}^{d\times d})$; which of course is not always appropriate as highlighted above.

Naturally, then, Dirichlet boundary conditions cannot be imposed – even before we could not impose Dirichlet boundary conditions on ν nor ∇y and "the original deformation y" is now forgotten, Therefore, *the specimen can only be loaded (and consequently deformed) by applying heat flux.*

As already in the non-convex case, we augment the system (6.1) with initial conditions 5.18

$$\nu_\varkappa(0,\cdot)=\nu_0,\qquad \lambda_\varkappa(0,\cdot)=\lambda_0,\qquad w_\varkappa(0,\cdot)=w_0=\widehat{c}_{\mathrm{v}}(\theta_0)\qquad \text{on } \Omega; \tag{6.2}$$

for simplification we assume the initial data to be *independent of* $\varkappa$.

Analogously as in Definition 5.4, we define weak solutions to (6.1) (with *fixed* $\varkappa$):

Definition 6.2. We shall call the triple $(\nu_\varkappa,\lambda_\varkappa,w_\varkappa)\in(\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d}))^{[0,T]}$ $\times W^{1,q}([0,T];L^q(\Omega;\mathbb{R}^{M+1}))\times(L^1([0,T];W^{1,1}(\Omega))\cap W^{1,1}([0,T];W^{1,\infty}(\Omega)^*))$ a weak solution of (6.1) with initial condition (6.2) if it satisfies

1. The **minimization principle**

$$\mathcal{G}^{\mathrm{C}}(\nu_\varkappa,\lambda_\varkappa(t),w_\varkappa(t))\le\mathcal{G}^{\mathrm{C}}(\tilde\nu,\lambda_\varkappa(t),w_\varkappa(t)), \tag{6.3}$$

for any $\tilde\nu\in\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d})$ and all $t\in[0,T]$.

2. The **flow rule** (5.23) with (ν,λ,w) replaced by $(\nu_\varkappa,\lambda_\varkappa,w_\varkappa)$.

3. The **enthalpy equation**

$$\begin{aligned}\int_Q\mathcal{K}(\lambda_\varkappa,w_\varkappa)\nabla w\cdot\nabla\zeta-w_\varkappa\dot\zeta\,\mathrm{d}x\,\mathrm{d}t+\int_\Omega w_\varkappa(T)\zeta(T)\,\mathrm{d}x+\int_\Sigma b\Theta(w_\varkappa)\zeta\,\mathrm{d}S\,\mathrm{d}t=\int_\Omega w_0\zeta(0)\,\mathrm{d}x\\ +\int_\Sigma b\theta_{\mathrm{ext}}\zeta\,\mathrm{d}S\,\mathrm{d}t+\int_Q\Big(\delta_S^*(\dot\lambda_\varkappa)+\alpha|\dot\lambda_\varkappa|^q+\big(\Theta(w_\varkappa)-\theta_{\mathrm{tr}}\big)\vec a\cdot\dot\lambda_\varkappa\Big)\zeta\,\mathrm{d}x\,\mathrm{d}t,\end{aligned} \tag{6.4}$$

for any $\zeta\in C^1(\bar Q)$.[3]

4. The remaining **initial conditions** in (6.2): $\nu_\varkappa(0,\cdot)=\nu_0$ and $\lambda_\varkappa(0,\cdot)=\lambda_0$ in Ω.

[2] Here already the enthalpy transformation has been performed.

[3] Note that this definition of very weak solutions to (6.1c)-(6.1d) is slightly stronger than the one

6.2 Existence analysis in the convex case

Since the *convex* system (6.1) is rather a simplification of the system in (5.17) it can be expected that existence of solutions can be proved in the convex case, too; the following theorem specifies this statement.

Theorem 6.3. [4] *Let (A1), (A3)-(A7) hold, $\varkappa$ be fixed. Then at least one weak solution $(\nu_\varkappa, \lambda_\varkappa, w_\varkappa)$ to the problem (6.1) in accord with Definition 6.2 does exist. Moreover, some of these solutions satisfy also*

$$\sup_{t\in[0,T]} \int_\Omega |\cdot|^p \bullet \nu_\varkappa \,\mathrm{d}x \le C, \tag{6.5}$$

$$\sup_{t\in[0,T]} \mathcal{Q}_\varkappa(\lambda_\varkappa - L\bullet\nu_\varkappa) \le C \tag{6.6}$$

$$\big\|\dot\lambda_\varkappa\big\|_{L^q(Q;\mathbb{R}^{M+1})} \le C, \tag{6.7}$$

$$\big\|w_\varkappa\big\|_{L^\infty([0,T];L^1(\Omega))} \le C, \tag{6.8}$$

$$\big\|\nabla w_\varkappa\big\|_{L^r(Q;\mathbb{R}^d)} \le C_r \qquad \text{with any } \ 1 \le r < \frac{d+2}{d+1}, \tag{6.9}$$

$$\big\|\dot w_\varkappa\big\|_{\mathcal{M}([0,T];W^{1,\infty}(\Omega)^*)} \le C. \tag{6.10}$$

for some constant C independent *of $\varkappa$.*

To prove Theorem 6.3, we follow the procedure of the proof Proposition 5.9 and discretize the system (6.1) by the backward Euler method, with (6.3) and (5.23) expressed by *one time-incremental minimization problem* (6.11)[5]; we call the triple $(\nu^k_{\varkappa,\tau}, \lambda^k_{\varkappa,\tau}, w^k_{\varkappa,\tau}) \in \mathcal{Y}^p(\Omega;\mathbb{R}^{d\times d}) \times L^{2q}(\Omega;\mathbb{R}^{M+1}) \times W^{1,2}(\Omega)$, the *discrete weak solution* of (6.1) at time-level k, $k = 1\dots T/\tau$, if it solves:

$$\left.\begin{aligned} &\text{Minimize} \quad \mathcal{G}^{\mathrm{C}}(k\tau,\nu,\lambda,\Theta(w^{k-1}_{\varkappa,\tau})) + \tau\int_\Omega |\lambda|^{2q} + \rho_q\Big(\frac{\lambda-\lambda^{k-1}_{\varkappa,\tau}}{\tau}\Big)\,\mathrm{d}x \\ &\text{subject to} \quad (\nu,\lambda) \in \mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d}) \times L^{2q}(\Omega;\mathbb{R}^{d+1}). \end{aligned}\right\} \tag{6.11}$$

and

$$\begin{aligned} \int_\Omega \frac{w^k_{\varkappa,\tau}-w^{k-1}_{\varkappa,\tau}}{\tau}\varphi + \mathcal{K}(\lambda^k_{\varkappa,\tau}, w^k_{\varkappa,\tau})\nabla w^k_{\varkappa,\tau}\nabla\varphi\,\mathrm{d}x + \int_\Gamma b^k_\tau \Theta(w^k_{\varkappa,\tau})\varphi\,\mathrm{d}S \\ = \int_\Omega \varrho_q\Big(\frac{\lambda^k_{\varkappa,\tau}-\lambda^{k-1}_{\varkappa,\tau}}{\tau}\Big)\varphi\,\mathrm{d}x + \int_\Omega \Theta(w^k_{\varkappa,\tau})\cdot\Big(\frac{\lambda^k_{\varkappa,\tau}-\lambda^{k-1}_{\varkappa,\tau}}{\tau}\Big)\varphi\,\mathrm{d}x + \int_\Gamma \theta_{\mathrm{ext}}\varphi\,\mathrm{d}S \end{aligned} \tag{6.12}$$

for all $\varphi \in W^{1,2}(\Omega;\mathbb{R})$. The initial conditions are satisfied in the sense that

$$\nu^0_{\varkappa,\tau} = \nu_0 \qquad \lambda^0_{\varkappa,\tau} = \lambda_{0,\tau} \qquad w^0_{\varkappa,\tau} = w_{0,\tau} \text{ for a.a. } x \in \Omega, \tag{6.13}$$

where $\lambda_{0,\tau}$, $w_{0,\tau}$ are suitable approximations of the original initial data in (6.2); they are constructed the same way as in (5.41) and (5.42).

given in (5.24); in particular, the term $\int_\Omega w_\varkappa(T)\zeta(T)\,\mathrm{d}x$ is included and $\zeta(T)$ needs not be 0. We can afford to include this term, since we will be able to prove that there exist weak solutions to (6.1) such that $w \in W^{1,1}([0,T];W^{1,\infty}(\Omega)^*)$. In fact, we could have included this term in (5.24) as well, but it has been omitted for simplicity. In the convex case, on the other hand, it will be handy to keep this term as it will help us to establish the energy equality in Remark 6.7 that, in turn, will be used in Section 6.3.

[4] The proof Theorem 6.3 was essential given in (Benešová, Kružík and Roubíček, 2012), we follow this work here. However, we pay more attention to the a-priori estimates to obtain (6.5)-(6.10), which was not done in (Benešová, Kružík and Roubíček, 2012).

[5] Due to *convexity* we can indeed use *one* joint minimization problem like in the proof Proposition 5.9 and do not need two minimization problems like in the proof exposed in Section 5.5.

Proposition 6.4. *Let (A1), (A3)-(A7) hold, $\varkappa$ be fixed and let also $w^0_{\varkappa,\tau} \geq 0$. Then there exists a discrete weak solution of (6.1) satisfying (6.11)-(6.12) such that $w^k_{\varkappa,\tau} \geq 0$ for all $k = 1 \dots T/\tau$.*

Moreover, the piecewise constant/affine interpolants of these discrete weak solutions defined as

$$\begin{aligned}\big[\bar\nu_{\varkappa,\tau}, \bar\lambda_{\varkappa,\tau}, \bar w_{\varkappa,\tau}\big](t) &= \big(\nu^k_{\varkappa,\tau}, \lambda^k_{\varkappa,\tau}, w^k_{\varkappa,\tau}\big),\\ \big[\lambda_{\varkappa,\tau}, w_{\varkappa,\tau}\big](t) &= \frac{t-(k-1)\tau}{\tau}\big(\lambda^k_{\varkappa,\tau}, w^k_{\varkappa,\tau}\big) + \frac{k\tau - t}{\tau}\big(\lambda^{k-1}_{\varkappa,\tau}, w^{k-1}_{\varkappa,\tau}\big),\end{aligned}$$

for $(k-1)\tau < t \leq k\tau$ and $k = 1, ..., T/\tau$, satisfy the following bounds:

$$\sup_{t\in[0,T]} \int_\Omega |\cdot|^p \bullet \bar\nu_{\varkappa,\tau}\,\mathrm{d}x \leq C, \tag{6.14}$$

$$\sup_{t\in[0,T]} \mathcal{Q}_\varkappa(\bar\lambda_{\varkappa,\tau} - L \bullet \bar\nu_{\varkappa,\tau}) \leq C \tag{6.15}$$

$$\big\|\dot\lambda_{\varkappa,\tau}\big\|_{L^q(Q;\mathbb{R}^{M+1})} \leq C, \tag{6.16}$$

$$\big\|\bar\lambda_{\varkappa,\tau}\big\|_{L^\infty([0,T];L^{2q}(\Omega;\mathbb{R}^{M+1}))} \leq C\tau^{-1/2q}, \tag{6.17}$$

$$\big\|\bar w_{\varkappa,\tau}\big\|_{L^\infty([0,T];L^1(\Omega))} \leq C, \tag{6.18}$$

$$\big\|\nabla \bar w_{\varkappa,\tau}\big\|_{L^r(Q;\mathbb{R}^d)} \leq C_r \qquad \text{with any } \ 1 \leq r < \frac{d+2}{d+1}, \tag{6.19}$$

$$\big\|\dot w_{\varkappa,\tau}\big\|_{\mathcal{M}([0,T];W^{1,\infty}(\Omega)^*)} \leq C, \tag{6.20}$$

with C independent of τ and κ.

Also, within the proof, we shall use the notion of "retarded" interpolants $\underline{w}_{\varkappa,\tau}$, $\underline{\nu}_{\varkappa,\tau}$ defined analogously to (5.110).

Proof. Similarly, as in (5.40), also in the convex case the discrete formulation is devised in such a way that (6.11) is decoupled from (6.12). Therefore, we first show existence of solutions to (6.12) – as in Proposition 5.9 or Lemma 5.14 we employ the *direct method* and the *convexity* of the cost function from(6.11) in λ as well as ν.[6]

Let us now prove the apriori estimates (6.14)-(6.20); to do so, we mimic the procedure of the proof Lemma 5.10. Indeed, we just have to slightly alter *Step 1* and *Step 2* of the proof Lemma 5.10 to get (6.14)-(6.18); having these estimates at our disposal, we can then show (6.19) and (6.20) *exactly* as in *Step 3* and *Step 4* in the proof Lemma 5.10, respectively.

Therefore, let us show that (6.14)-(6.18) uniformly in $\varkappa$ and τ. Similarly as when deriving (5.112), we may obtain the following energy inequality[7]

$$\begin{aligned}\int_\Omega \phi_1 \bullet \bar\nu_{\varkappa,\tau}(t_k)\,\mathrm{d}x + \mathcal{Q}_\varkappa\big(\bar\lambda_{\varkappa,\tau}(t_k) - L\bullet\bar\nu_{\varkappa,\tau}(t_k)\big)&\\ \leq \int_\Omega \phi_1 \bullet \nu_0\,\mathrm{d}x + \int_0^{t_k}\int_\Omega \mathcal{Q}'_\varkappa\big(\bar\lambda_{\varkappa,\tau} - L\bullet\bar\nu_{\varkappa,\tau}\big)\cdot\dot\lambda_{\varkappa,\tau}\,\mathrm{d}x\,\mathrm{d}t.&\end{aligned} \tag{6.21}$$

Also, as in (5.58), we may derive the discrete flow-rule by setting the partial subdifferential with respect to λ of the cost function in (6.11) at λ^l_τ to zero and summing

[6] Cf. also the proof Lemma 5.14 for more details on how to handle the Young measure.

[7] I.e. we need to test (6.11) in the l-th step by $(\nu^{l-1}_{\varkappa,\tau}, \lambda^l_{\varkappa,\tau})$ and sum from 1 to k.

from 1 to k; i.e. we have

$$\int_0^{t_k}\!\!\int_\Omega \rho_q(\dot\lambda_{\varkappa,\tau})\,\mathrm{d}x\,\mathrm{d}t \le \int_0^{t_k}\!\!\int_\Omega \Big(\mathcal{Q}'_\varkappa(\bar\lambda_{\varkappa,\tau}-L\bullet\bar\nu_{\varkappa,\tau})\cdot(v_{\varkappa,\tau}-\dot\lambda_{\varkappa,\tau})+\rho_q(v_{\varkappa,\tau} + \big(\Theta(\underline{w}_{\varkappa,\tau})-\theta_{\rm tr}\big)\vec a\cdot(v_{\varkappa,\tau}-\dot\lambda_{\varkappa,\tau})+2q\tau|\bar\lambda_{\varkappa,\tau}|^{2q-2}\bar\lambda_{\varkappa,\tau}(v_{\varkappa,\tau}-\dot\lambda_{\varkappa,\tau})\Big)\Big)\,\mathrm{d}x\,\mathrm{d}t, \tag{6.22}$$

where $v_{\varkappa,\tau}$ is an arbitrary test function such that $v_{\varkappa,\tau}(\cdot,x)$ is piecewise constant on the intervals $(t_{j-1},t_j]$ and $v_{\varkappa,\tau}(t_j,\cdot)\in L^{2q}(\Omega;\mathbb{R}^{d+1})$ for every j. Further, setting $v_{\varkappa,\tau}=0$ and employing the discrete chain rule as in (5.47) gives

$$\int_0^{t_k}\!\!\int_\Omega \rho_q(\dot\lambda_{\varkappa,\tau})\,\mathrm{d}x\,\mathrm{d}t + 2q\tau\int_\Omega|\bar\lambda_{\varkappa,\tau}(t_k)|^{2q}\,\mathrm{d}x \le \int_0^{t_k}\!\!\int_\Omega \Big(\mathcal{Q}'_\varkappa(\bar\lambda_{\varkappa,\tau}-L\bullet\bar\nu_{\varkappa,\tau})\cdot(-\dot\lambda_{\varkappa,\tau}) + \big(\Theta(\underline{w}_{\varkappa,\tau})-\theta_{\rm tr}\big)\vec a\cdot(-\dot\lambda_{\varkappa,\tau})\Big)\,\mathrm{d}x\,\mathrm{d}t + 2q\tau\int_\Omega|\bar\lambda_{\varkappa,\tau}(0)|^{2q}, \tag{6.23}$$

Now adding (6.23) and (6.21) gives the following inequality

$$\int_\Omega \phi_1\bullet\bar\nu_{\varkappa,\tau}(t_k)+2q\tau|\bar\lambda_{\varkappa,\tau}(t_k)|^{2q}\,\mathrm{d}x + \mathcal{Q}_\varkappa(\bar\lambda_{\varkappa,\tau}(t_k)-L\bullet\bar\nu_{\varkappa,\tau}(t_k))+\int_0^{t_k}\!\!\int_\Omega\rho_q(\dot\lambda_{\varkappa,\tau})\,\mathrm{d}x\,\mathrm{d}t \le \int_\Omega\phi_1\bullet\bar\nu^0+2q\tau\int_\Omega|\bar\lambda_{\varkappa,\tau}(0)|^{2q}\,\mathrm{d}y\int_0^{t_k}\!\!\int_\Omega\big(\Theta(\underline{w}_{\varkappa,\tau})-\theta_{\rm tr}\big)\vec a\cdot(-\dot\lambda_{\varkappa,\tau})\,\mathrm{d}x\,\mathrm{d}t,$$

which, after using the Young inequality as in (5.47), leads to

$$\int_\Omega \phi_1\bullet\bar\nu_{\varkappa,\tau}(t_k)+2q\tau|\bar\lambda_{\varkappa,\tau}(t_k)|^{2q}\,\mathrm{d}x + \mathcal{Q}_\varkappa(\bar\lambda_{\varkappa,\tau}(t_k)-L\bullet\bar\nu_{\varkappa,\tau}(t_k))+\int_0^{t_k}\!\!\int_\Omega\rho_q(\dot\lambda_{\varkappa,\tau})\,\mathrm{d}x\,\mathrm{d}t \le C\int_0^{t_k}\!\!\int_\Omega|\underline{w}_{\varkappa,\tau}|\,\mathrm{d}x\,\mathrm{d}t+C, \tag{6.24}$$

with C *independent of* $\varkappa$ and τ.

Finally, summing the discrete version of the enthalpy equation (6.12) from 0 to k leads, similarly as when obtaining (5.76), to

$$\int_0^{t_k}\!\Big(\int_\Omega\big(\dot w_{\varkappa,\tau}\varphi+\mathcal{K}(\bar\lambda_{\varkappa,\tau},\bar w_{\varkappa,\tau})\nabla\bar w_{\varkappa,\tau}\cdot\nabla\varphi\big)\,\mathrm{d}x+\int_\Gamma\bar b_{\varkappa,\tau}\Theta(\bar w_{\varkappa,\tau})\varphi\,\mathrm{d}S\Big)\,\mathrm{d}t = \int_0^{t_k}\!\Big(\int_\Omega\big(\varrho_q(\dot\lambda_{\varkappa,\tau})+\Theta(\bar w_{\varkappa,\tau})\vec a\cdot\dot\lambda_{\varkappa,\tau}\big)\varphi\,\mathrm{d}x+\int_\Gamma\bar b_{\varkappa,\tau}\bar\theta_{{\rm ext},\tau}\varphi\,\mathrm{d}S\Big)\,\mathrm{d}t, \tag{6.25}$$

where φ is an arbitrary test function, such that $\varphi(\cdot,x)$ is piecewise constant on the intervals $(t_{j-1},t_j]$ and $\varphi(t_j,\cdot)\in H^1(\Omega)$ for every j. In the same spirit as in (5.79), we test equation (6.25) by 1 and estimate the right-hand side by exploiting the Young inequality to get

$$\int_0^{t_k}\!\!\int_\Omega\dot w_{\varkappa,\tau}(t,x)\,\mathrm{d}x+\int_\Gamma\bar b_{\varkappa,\tau}\Theta(\bar w_{\varkappa,\tau})\,\mathrm{d}S\,\mathrm{d}t\le\int_Q 2\alpha|\dot\lambda_{\varkappa,\tau}|^q+C|\bar w_{\varkappa,\tau}|\,\mathrm{d}x\,\mathrm{d}t.$$

Multiplying this by $\alpha/(8q)$ and adding to (6.24) already yields (6.14)–(6.18) by the usage of the discrete Gronwall inequality; note that these estimates are indeed *uniform in* $\varkappa$. □

Proposition 6.5 (Convergence for $\tau\to0$)**.** *Let the assumptions (A1), (A3)-(A7) hold,* $\varkappa$ *be fixed. Then there exist* $(\nu_\varkappa,\lambda_\varkappa,w_\varkappa)\in(\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d}))^{[0,T]}\times W^{1,q}([0,T];L^q(\Omega;\mathbb{R}^{M+1}))$

$\times L^r([0,T];W^{1,r}(\Omega))$ *and a sequence* $\tau \to 0$ *such that*

$$\bar{\lambda}_{\varkappa,\tau} \overset{*}{\rightharpoonup} \lambda_\varkappa \qquad \text{in } L^\infty([0,T];L^q(\Omega,\mathbb{R}^{M+1})) \tag{6.26}$$

$$\bar{\lambda}_{\varkappa,\tau}(t) \rightharpoonup \lambda_\varkappa(t) \qquad \forall t\in[0,T] \text{ in } L^q(\Omega;\mathbb{R}^{M+1}), \tag{6.27}$$

$$\dot{\lambda}_{\varkappa,\tau} \to \dot{\lambda}_\varkappa \qquad \text{in } L^q(Q;\mathbb{R}^{M+1}), \tag{6.28}$$

$$\bar{w}_{\varkappa,\tau} \rightharpoonup w_\varkappa \qquad L^r([0,T];W^{1,r}(\Omega)),\ r<\tfrac{d+2}{d+1} \text{ and } \bar{w}_{\varkappa,\tau}\to w_\varkappa \text{ in } L^1(Q), \tag{6.29}$$

with $(\lambda_{\varkappa,\tau},w_{\varkappa,\tau})$ *the piecewise affine interpolants and* $(\bar{\lambda}_{\varkappa,\tau},\bar{w}_{\varkappa,\tau})$ *the piecewise constant interpolants defined in Lemma 6.4.*
Moreover, for each $t\in[0,T]$ *there exists a subsequence* $\tau_{k(t)}$ *such that*

$$\bar{\nu}_{\varkappa,\tau_{k(t)}}(t) \overset{*}{\rightharpoonup} \nu(t) \quad \text{in } L^\infty_{\rm w}(\Omega;\mathcal{M}(\mathbb{R}^d)), \tag{6.30}$$

with $\bar{\nu}_{\varkappa,\tau}$ *defined again in Lemma 6.4.*

Every cluster point $(\nu_\varkappa,\lambda_\varkappa,w_\varkappa)$ *obtained in this way is then is a weak solution of (6.1) in accord with Definition 6.2 and satisfies (6.7)-(6.10).*

Remark 6.6. Note that the statement of Proposition 6.5 is indeed *stronger* than the statements of related Theorem 5.15 – while in Proposition 6.5 we claim that *every* cluster point of discrete solutions to (6.1) solves (6.1) weakly, in Theorem 5.15 we could prove an analogous statement only for *some* cluster points.

The reason is that in the *convex* case the vector of volume fraction $L\bullet\nu$ will be, for each λ, *uniquely defined* – this will help us to resolve the problems with measurability of $\mathcal{Q}'_\varkappa(\lambda_\varkappa - L\bullet\nu_\varkappa)\cdot(v-\dot{\lambda}_\varkappa)$ encountered in the proof Theorem 5.15 in a more straightforward way than in the mentioned proofs. In particular, we need not to reformulate the discrete flow-rule (6.22) as in *Step 1* of the proof Theorem 5.15, nor shall we employ Fatou's lemma.

Recall, that in order to perform the mentioned reformulation of the flow-rule, we needed to discretize the non-convex system (5.22) – (5.23) by *two* minimization problems; in the convex case, where there is no need to reformulate the flow-rule, *only one joint minimization problem* (6.11) suffices.

Proof. For clarity, let us divide the proof into several steps.

Step 1: Selection of subsequences, limit passage in the minimization principle for $\nu_\varkappa$
analogously to *Step 3* of the proof Proposition 5.9, we find, owing to (6.16)-(6.20), a subsequence of τ's (not relabeled) such that (6.26), (6.27), (6.29) and

$$\dot{\lambda}_{\varkappa,\tau} \overset{*}{\rightharpoonup} \dot{\lambda}_\varkappa \quad \text{in } L^q(Q;\mathbb{R}^{M+1}), \tag{6.31}$$

hold. Also, as in *Step 1* of Theorem 5.12, $\Theta(\bar{w}_{\varkappa,\tau})\to\Theta(w_\varkappa)$ in $L^{q'}(Q)$ and, due to (5.109), $\Theta(\underline{w}_{\varkappa,\tau})\to\Theta(w_\varkappa)$ in $L^{q'}(Q)$, too. Furthermore, due to a-priori estimate (6.20), we may also employ Helly's selection principle (cf. e.g. (Francfort and Mielke, 2006; Mielke and Theil, 2004)) to get even that

$$\bar{w}_{\varkappa,\tau}(t) \rightharpoonup w_\varkappa(t) \qquad \text{for all } t\in[0,T] \text{ weakly in } W^{1,r}(\Omega). \tag{6.32}$$

At last, due to (6.14) and (A3), there exists a $\Xi\in L^2(Q;\mathbb{R}^{d+1})$ such that

$$L\bullet\bar{\nu}_{\varkappa,\tau} \rightharpoonup \Xi \qquad \text{in } L^2(Q;\mathbb{R}^{d+1}). \tag{6.33}$$

Let us *fix some* $t\in[0,T]$. Exploiting again (5.104), select a subsequence of τ's labeled $\tau_{k(t)}$[8] such that $\bar{\nu}_{\varkappa,\tau_{k(t)}}(t) \rightharpoonup \nu_\varkappa(t)$ in $L^\infty_{\rm w}(\Omega;\mathcal{M}(\mathbb{R}^d))$; due (5.104) $\nu(t)\in$

[8] As indicated by the index $k=k(t)$, this selection *may depend on time* t.

$\mathcal{Y}^p(\Omega;\mathbb{R}^{d\times d})$[9]. Since L is bounded (cf. (A3)), it holds also that $L\bullet\bar\nu_{\varkappa,\tau_{k(t)}}(t)\rightharpoonup L\bullet\nu_\varkappa(t)$ in $L^2(\Omega;\mathbb{R}^{d+1})$; realize that this *does not* imply that $L\bullet\nu_\varkappa=\Xi$.

Due to the weak lower semi-continuity of the norms any selected cluster point $(\nu_\varkappa,\lambda_\varkappa,\nu_\varkappa)$ preserves the bounds (6.7)-(6.10).

As to establishing (6.3), note that a direct consequence of (6.11) is the *discrete minimization principle* that reads as

$$\int_\Omega\phi_1\bullet\bar\nu_{\varkappa,\tau_{k(t)}}(t)\,\mathrm{d}x+\mathcal{Q}_\varkappa\big(\bar\lambda_{\varkappa,\tau_{k(t)}}(t)-L\bullet\bar\nu_{\varkappa,\tau_{k(t)}}(t)\big)\le\int_\Omega\phi_1\bullet\hat\nu\,\mathrm{d}x+\mathcal{Q}_\varkappa\big(\bar\lambda_{\varkappa,\tau_{k(t)}}(t)-L\bullet\hat\nu\big)\tag{6.34}$$

for any $\hat\nu\in\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d})$. By applying $\liminf_{\tau_{k(t)}\to0}$ on both sides, we indeed get (6.11)[10].

Furthermore, due to the *convexity* of Young measures and the *strict convexity* of $\mathcal{Q}_\varkappa(\cdot)$[11], $L\bullet\nu_\varkappa$, with $\nu_\varkappa$ some solutions of (6.3) corresponding to the already selected $\lambda_\varkappa=\lambda_\varkappa(t)$, is *determined uniquely* although the minimizer $\nu_\varkappa$ itself does not need to be.[12]

In turn it means that $L\bullet\bar\nu_{\varkappa,\tau}(t)\rightharpoonup L\bullet\nu_\varkappa(t)$ in $L^2(\Omega;\mathbb{R}^{d+1})$ *same* sub-sequence of τ's for which (6.26), (6.27), (6.29) and (6.31) hold; in particular *this subsequence is not time-dependent*. Hence, by usage of the Lebesgue dominated convergence theorem, $L\bullet\nu_\varkappa(t)=\Xi(t)$ and thus $L\bullet\nu_\varkappa$ is measurable.

Step 2: Limit passage in the flow-rule and strong convergence of $\dot\lambda_{\varkappa,\tau}$
Having selected subsequences and having established (6.3), we shall pass to the limit $\liminf_{\tau\to0}$ in the discrete flow-rule (6.22). As already in the proof Theorem 5.12 and Theorem 5.15, we expect the most difficulties in the term $\mathcal{Q}'_\varkappa\big(\bar\lambda_{\varkappa,\tau}-L\bullet\bar\nu_{\varkappa,\tau}\big)\cdot\big(v_{\varkappa,\tau}-\dot\lambda_{\varkappa,\tau}\big)$ since in all other terms in (6.22) we can pass to the limit the same way as in *Step 4* of the proof Proposition 5.9.

However, in the convex case, finding $\lim_{\tau\to0}\mathcal{Q}'_\varkappa\big(\bar\lambda_{\varkappa,\tau}-L\bullet\bar\nu_{\varkappa,\tau}\big)\cdot\big(v_\tau-\dot\lambda_\tau\big)$ is straightforward because we know that $L\bullet\bar\nu_{\varkappa,\tau}(t)\rightharpoonup L\bullet\nu_\varkappa(t)$ *weakly* in $L^2(\Omega;\mathbb{R}^{M+1})$ for some a subsequence of τ's *independent* of t[13] and hence, as $\mathcal{Q}_\varkappa(\cdot)$ is compact (cf. (5.2), (5.3)), we get

$$\lim_{\tau\to0}\mathcal{Q}'_\varkappa\big(\bar\lambda_{\varkappa,\tau}(t)-L\bullet\bar\nu_{\varkappa,\tau}(t)\big)\cdot\big(v_{\varkappa,\tau}(t)-\dot\lambda_{\varkappa,\tau}(t)\big)=\mathcal{Q}'_\varkappa\big(\lambda_\varkappa(t)-L\bullet\nu_\varkappa(t)\big)\cdot\big(v(t)-\lambda_\varkappa(t)\big),\tag{6.35}$$

for all $t\in[0,T]$; hence, we are entitled to use Lebesgue's dominated convergence theorem (note that the sequence is actually dominated by constant owing to estimates (6.14)–(6.16)) to get that $\mathcal{Q}'_\varkappa\big(\bar\lambda_{\varkappa,\tau}-L\bullet\bar\nu_{\varkappa,\tau}\big)\cdot\big(v_{\varkappa,\tau}-\dot\lambda_{\varkappa,\tau}\big)\to\mathcal{Q}'_\varkappa\big(\lambda_\varkappa-L\bullet\nu_\varkappa\big)\cdot\big(v-\lambda_\varkappa\big)$ in $L^1([0,T])$. Combining all above said, we get (5.23). Furthermore, we show (6.28) by

[9] This can be shown e.g. thanks to Proposition 2.10.

[10] We proceed analogously to *Step 2* in Theorem 5.12.

[11] Recall, that due to its definition in (5.2), $\mathcal{Q}_\varkappa(\cdot)$ is essentially *quadratic*.

[12] To see this, suppose that there existed two solutions of (6.3) $[\nu_\varkappa]_1$ and $[\nu_\varkappa]_2$ such that $L\bullet[\nu_\varkappa]_1\neq L\bullet[\nu_\varkappa]_2$. Then, due the strict convexity of $\mathcal{Q}_\varkappa(\cdot)$ it held for $\nu_\varkappa=\frac12[\nu_\varkappa]_1+\frac12[\nu_\varkappa]_2\in\mathcal{Y}^p(\Omega;R^{d\times d})$

$$\begin{aligned}\int_\Omega\phi_1\nu_\varkappa\,\mathrm{d}x+\mathcal{Q}_\varkappa(\lambda(t)-L\bullet\nu_\varkappa)<{}&\frac12\Big(\int_\Omega\phi_1[\nu_\varkappa]_1\,\mathrm{d}x+\mathcal{Q}_\varkappa(\lambda(t)-L\bullet[\nu_\varkappa]_1)\Big)\\&+\frac12\Big(\int_\Omega\phi_1[\nu_\varkappa]_2\,\mathrm{d}x+\mathcal{Q}_\varkappa(\lambda(t)-L\bullet[\nu_\varkappa]_2)\Big),\end{aligned}$$

which yields a contradiction, since the expression on the right-hand side is *equal* to the minimum of $\int_\Omega\phi_1\tilde\nu\,\mathrm{d}x+\mathcal{Q}_\varkappa(\lambda(t)-L\bullet\tilde\nu)$ over all $\tilde\nu\in\mathcal{Y}^p(\Omega;R^{d\times d})$.

[13] Recall that we *were not able* to get an analogous statement in the non-convex case.

mimicking the procedure of *Step 5* in the proof Proposition 5.9 – i.e. we test (6.22) *reformulated using the convexity of* $|\cdot|^q$ by $\dot\lambda_{\mathrm{S},\varkappa,\tau}$, a piecewise constant approximation of the function $\dot\lambda_\varkappa$ such that $\dot\lambda_{\mathrm{S},\varkappa,\tau}\to\dot\lambda_\varkappa$ strongly in $L^q(Q;\mathbb{R}^{M+1})$ and moreover $\|\dot\lambda_{\mathrm{S},\varkappa,\tau}\|_{L^{2q}(Q;\mathbb{R}^{M+1})}\le C\tau^{-1/(2q+1)}$, further we test (5.23) by $\dot\lambda_{\varkappa,\tau}$ and add the two obtained inequalities. When passing to the limit $\tau\to0$, we rely on (6.35).

Step 3: Enthalpy equation:
For limit passage in the discrete enthalpy equation, we first perform by-parts integration in (6.12) to get

$$-\int_0^T\Big(\int_\Omega \bar w_{\varkappa,\tau}\dot{\bar\varphi}+\mathcal{K}(\bar\lambda_{\varkappa,\tau},\bar w_{\varkappa,\tau})\nabla\bar w_{\varkappa,\tau}\nabla\bar\varphi\,\mathrm{d}x+\int_\Gamma \bar b_\tau\Theta(\bar w_{\varkappa,\tau})\bar\varphi\,\mathrm{d}S\Big)\,\mathrm{d}t+\int_\Omega \bar w_{\varkappa,\tau}(T)\bar\varphi(T)$$
$$=\int_\Omega \bar w_{\varkappa,\tau}(0)\bar\varphi(0)\,\mathrm{d}x+\int_0^{t_k}\Big(\int_\Omega\big(\varrho_q(\dot\lambda_{\varkappa,\tau})+\Theta(\bar w_{\varkappa,\tau})\vec a\cdot\dot\lambda_{\varkappa,\tau}\big)\bar\varphi\,\mathrm{d}x+\int_\Gamma \bar b_\tau\bar\theta_{\mathrm{ext},\tau}\bar\varphi\,\mathrm{d}S\Big)\,\mathrm{d}t,$$

for all $\bar\varphi$ piecewise constant on the intervals $(t_{j-1},t_j]$ such that, for any j, $\bar\varphi(t_j,\cdot)\in W^{1,2}(\Omega)$ and φ piecewise linear on the intervals $(t_{j-1},t_j]$, such that $\bar\varphi(t_j,\cdot)=\varphi(t_j,\cdot)$.

Then, we proceed analogously to *Step 7* of the proof Proposition 5.9; only for the term $\int_\Omega \bar w_{\varkappa,\tau}(T)\bar\varphi(T)\,\mathrm{d}x$ we exploit (6.32).

□

Remark 6.7 (Total energy balance). Let us note that, by a similar technique as in *Step 6*, we can establish, from (6.11), the *mechanic energy equality* that reads as[14]

$$\int_\Omega \phi_1\bullet\nu_\varkappa(T)\,\mathrm{d}x+\mathcal{Q}_\varkappa\big(\lambda_\varkappa(T)-L\bullet\nu_\varkappa(T)\big)$$
$$=\int_\Omega\phi_1\bullet\nu_0\,\mathrm{d}x+\mathcal{Q}_\varkappa\big(\lambda_0-L\bullet\nu_0\big)+\int_Q\mathcal{Q}'_\varkappa(\lambda_\varkappa-L\bullet\nu_\varkappa)\cdot\dot\lambda_\varkappa\,\mathrm{d}x\,\mathrm{d}t.\qquad(6.36)$$

Furthermore, let us rewrite the flow-rule (5.23) using *convexity of* $|\cdot|^q$ as

$$\int_Q\big(\Theta(w)_\varkappa-\theta_{\mathrm{tr}}\big)\vec a\cdot\big(v-\dot\lambda_\varkappa\big)+\delta_S^*(v)+\mathcal{Q}'_\varkappa\big(\lambda_\varkappa-L\bullet\nu_\varkappa\big)\cdot(v-\dot\lambda_\varkappa)+\alpha|\dot\lambda|^{q-2}\dot\lambda\cdot(v-\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t$$
$$\ge\int_Q\delta_S^*(\dot\lambda_\varkappa)\,\mathrm{d}x\,\mathrm{d}t;$$

testing this by 0 and also by $2\dot\lambda$ gives, relying on one-homogeneity of $\delta_S^*(\cdot)$

$$\int_Q\delta_S^*(\dot\lambda_\varkappa)+\alpha|\dot\lambda_\varkappa|^q+\big(\Theta(w_\varkappa)-\theta_{\mathrm{tr}}\big)\vec a\cdot\dot\lambda_\varkappa\,\mathrm{d}x\,\mathrm{d}t+$$
$$=-\int_Q\mathcal{Q}'_\varkappa\big(\lambda_\varkappa-L\bullet\nu_\varkappa\big)\cdot\dot\lambda_\varkappa\,\mathrm{d}x\,\mathrm{d}t$$
$$=-\int_\Omega\phi_1\bullet\nu_\varkappa(T)\,\mathrm{d}x-\mathcal{Q}_\varkappa\big(\lambda_\varkappa(T)-L\bullet\nu_\varkappa(T)\big)+\int_\Omega\phi_1\bullet\nu_0\,\mathrm{d}x+\mathcal{Q}_\varkappa\big(\lambda_0-L\bullet\nu_0\big),$$

[14] The mentioned technique relies on approximating the Lebesgue integral by Riemann sums. In particular, we introduce a partition of the interval $[0,T]$ $0=t_0^\beta\le t_1^\beta\le t_2^\beta\dots t_{N(\beta)}^\beta=T$ with $\max_{i=1\dots N(\beta)}(t_i+t_{i-1})=\beta$ and exploit in each point (6.11) two times. First, we use (6.11) at the time-step t_k^β and test it by $\nu_\varkappa(t_{k-1}^\beta)$, secondly we test (6.11) at the time-step t_{k-1}^β by $\nu_\varkappa(t_k^\beta)$. Then, we sum both obtained inequalities from 1 to $N(\beta)$ and pass to the limit $\beta\to0$ exploiting (Dal Maso et al., 2005, Lemma 4.12).

where in the last equality we exploited (6.36). Finally, plugging this expression into the weak enthalpy equation tested (6.4) by 1

$$\int_\Omega w_\varkappa(T)\,\mathrm{d}x+\int_\Sigma b\Theta(w_\varkappa)\,\mathrm{d}S\,\mathrm{d}t-\int_\Omega w_0\,\mathrm{d}x-\int_\Sigma b\theta_{\mathrm{ext}}\,\mathrm{d}S\,\mathrm{d}t \\ +\int_Q\Big(\delta_S^*(\dot\lambda_\varkappa)+\alpha|\dot\lambda_\varkappa|^q+\Theta(w_\varkappa)\vec a\cdot\dot\lambda_\varkappa\Big)\,\mathrm{d}x\,\mathrm{d}t,$$

yields the *total energy balance*

$$\int_\Omega w_\varkappa(T)\,\mathrm{d}x+\int_\Sigma b\Theta(w_\varkappa)\,\mathrm{d}S\,\mathrm{d}t-\int_\Omega w_0\,\mathrm{d}x-\int_\Sigma b\theta_{\mathrm{ext}}\,\mathrm{d}S\,\mathrm{d}t-\int_Q\theta_{\mathrm{tr}}\vec a\cdot\dot\lambda_\varkappa \\ =\int_\Omega -\phi_1\bullet\nu_\varkappa(T)+\phi_1\bullet\nu_0\,\mathrm{d}x-\mathcal{Q}_\varkappa\big(\lambda_\varkappa(T)-L\bullet\nu_\varkappa(T)\big)+\mathcal{Q}_\varkappa\big(\lambda_0-L\bullet\nu_0\big). \tag{6.37}$$

We shall exploit this balance in Section 6.3 below.

6.3 The limit $\varkappa\to\infty$

In the convex case, we can *justify* the penalty approach from Section 5.1.1, i.e. we can show that, if $\varkappa\to\infty$, (weak) solutions the system (6.1) converge to (very weak)[15] solutions of the following system:

$$\left.\begin{array}{ll}\text{minimize} & \displaystyle\int_\Omega\phi_1\bullet\nu\,\mathrm{d}x\\ \text{subject to} & \nu\in\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d}) \text{ such that } L\bullet\nu=\lambda\\ & \text{with } (\lambda,\theta) \text{ fixed solutions of (6.38b), (6.38c),}\end{array}\right\}\ \text{for a.a. } t\in[0,T], \tag{6.38a}$$

$$\partial\delta_S^*(\dot\lambda)+\partial\delta_{\{\lambda=L\bullet\nu\}}(\lambda)+\alpha|\dot\lambda|^{q-2}\dot\lambda+\Theta(w)\vec a\ni\theta_{\mathrm{tr}}\vec a \qquad \text{in } Q, \tag{6.38b}$$

$$\dot w-\mathrm{div}(\mathcal{K}(\lambda,w)\nabla w)=\delta_S^*(\dot\lambda)+\alpha|\dot\lambda|^q+\Theta(w)\dot\lambda \qquad \text{in } Q, \tag{6.38c}$$

$$\big(\mathcal{K}(\lambda,w)\nabla w\big)\cdot n+b\Theta(w)=b\theta_{\mathrm{ext}} \qquad \text{on } \Sigma. \tag{6.38d}$$

The system is completed by initial conditions (6.2) that, however, are *compatible* in the sense that $\lambda_0=L\bullet\nu_0$.

In (6.38), contrary to (5.17) or (5.28), λ *plays not the role of a phase-field* anymore – since we are able to to prove that $\lambda=L\bullet\nu$ and not just $\lambda\sim L\bullet\nu$, λ *indeed* now corresponds to the vector of volume fractions stemming from microstructure.

Remark 6.8. Note that (6.38a) is weaker than the corresponding minimization problem including the penalty (6.1a) – indeed in (6.1a) we need the solution to be a minimizer for *all* $t\in[0,T]$, in (6.38a) this is required only for a.a. t. This is due to the fact that in the proof Theorem 6.13 (below) we will only be able to show that $\mathcal{Q}_\varkappa(\lambda_\varkappa(t)-L\bullet\nu_\varkappa(t))\to0$ only for a.a. $t\in[0,T]$.

For simplicity, we shall assume, within this subsection, that $q=2$ and prescribe a *specific form for the penalty functional* $\mathcal{Q}_\varkappa$, namely we set $\mathfrak{Q}=\nabla\Delta^{-1}$ in (5.2) which makes $\big(\int_\Omega|\mathfrak{Q}\cdot|^2\big)^{1/2}$ an equivalent norm in $H^{-1}(\Omega;\mathbb{R}^{M+1})$ (Benešová, Kružík and Roubíček, 2012). We shall also use the following abbreviation for the scalar product for $a,b\in H^{-1}(\Omega;\mathbb{R}^{M+1})$

$$\langle\!\langle a,b\rangle\!\rangle=\int_\Omega(\mathfrak{Q}a)\cdot(\mathfrak{Q}b)\,\mathrm{d}x; \tag{6.39}$$

[15] We use here the adjective "very weak" in order to emphasize that the devised weak formulation of (6.38a) in Definition 6.9 will be even weaker than the one in Definition 6.2 for 6.1a.

note that with this notation, owing to (5.2), (5.3),

$$\int_\Omega \mathcal{Q}'_\varkappa(a)\cdot b\,\mathrm{d}x = \varkappa\langle\!\langle a,b\rangle\!\rangle.$$

First, let us give a *weak formulation*; an essential difference to the penalized situation is that now (6.38b) is a *doubly nonlinear* problem. Finding weak formulations of such kind of problems is usually not trivial, here we rely on the reformulation of the flow rule the using mechanic energy (in)equality as in *Step 1* of the proof Theorem 5.12 and combine the standard definitions for both sub-differentials.

Definition 6.9. We shall call the triple $(\nu,\lambda,w)\in(\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d}))^{[0,T]}\times W^{1,q}([0,T];L^q(\Omega;\mathbb{R}^{M+1}))\times L^1([0,T];W^{1,1}(\Omega))$ such that $\lambda = L\bullet\nu$ for a.a. $t\in[0,T]$ and a.e. on Ω a weak solution of (6.1a) with initial condition (6.2) if it satisfies:

1. The **minimization principle**

$$\int_\Omega \phi_1\bullet\nu\,\mathrm{d}x \le \int_\Omega \phi_1\bullet\tilde\nu\,\mathrm{d}x \tag{6.40}$$

for any $\tilde\nu\in\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d})$ such that $\lambda = L\bullet\tilde\nu$ and a.a. $t\in[0,T]$ and for $t=T$.

2. The **flow rule**

$$\begin{aligned}\int_Q \rho_q(\dot\lambda)\,\mathrm{d}x \le{}& \int_0^T \langle\!\langle \mathfrak{s}, v\rangle\!\rangle + \int_Q (\Theta(w)-\theta_{\mathrm{tr}})\vec a\cdot(v-\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t\\ &+\int_Q \rho_q(v)\,\mathrm{d}x\,\mathrm{d}t - \int_\Omega \Big(\phi_1\bullet\nu(T)-\phi_1\bullet\nu_0\Big)\,\mathrm{d}x \qquad \forall v\in L^2(Q;\mathbb{R}^{M+1})\end{aligned} \tag{6.41}$$

with $\mathfrak{s}\in L^2([0,T];H^{-1}(\Omega;\mathbb{R}^{M+1}))$ defined through

$$\begin{aligned}0\int_0^T \ge \langle\!\langle \mathfrak{s}, \mathfrak{v}-\lambda\rangle\!\rangle\,\mathrm{d}t \qquad & \forall\,\mathfrak{v}\in L^2(Q;\mathbb{R}^{M+1}) \text{ such that } \mathfrak{v}(t,x) = L\bullet\nu_x(t)\\ & \text{for a.a. } t\in[0,T] \text{ a.e. on } \Omega.\end{aligned} \tag{6.42}$$

3. The **enthalpy inequality**

$$\begin{aligned}\int_Q \mathcal{K}(\lambda,w)\nabla w\cdot\nabla\zeta - w\dot\zeta\ \mathrm{d}x\,\mathrm{d}t + \int_\Sigma b\Theta(w)\zeta\ \mathrm{d}S\,\mathrm{d}t + \int_\Omega w(T)\zeta(T) - \int_\Omega w_0\zeta(0)\ \mathrm{d}x\\ \ge \int_\Sigma b\theta_{\mathrm{ext}}\zeta\ \mathrm{d}S\,\mathrm{d}t + \int_Q \Big(\delta_S^*(\dot\lambda)+\alpha|\dot\lambda|^q+\Theta(w)\vec a\cdot\dot\lambda\Big)\zeta\ \mathrm{d}x\,\mathrm{d}t,\end{aligned} \tag{6.43}$$

for any $\zeta\in C^1(\bar Q)$ such that $\zeta\ge 0$ on $\bar Q$.

4. The **the total energy balance**:

$$\begin{aligned}\int_\Omega w(T)\ \mathrm{d}x + \int_\Sigma b\Theta(w)\ \mathrm{d}S\,\mathrm{d}t + \int_\Omega -\phi_1\bullet\nu(T) - \int_Q \theta_{\mathrm{tr}}\vec a\cdot\dot\lambda\,\mathrm{d}x\,\mathrm{d}t\\ = \int_\Omega w_0\ \mathrm{d}x + \int_\Sigma b\theta_{\mathrm{ext}}\ \mathrm{d}S\,\mathrm{d}t \int_\Omega \phi_1\bullet\nu_0\,\mathrm{d}x.\end{aligned} \tag{6.44}$$

5. The remaining **initial conditions**: $\nu(0,\cdot)=\nu_0$ and $\lambda(0,\cdot)=\lambda_0$; compatible in the sense that $\lambda_0 = L\bullet\nu_0$.

Remark 6.10 (Selectivity). Note that the Definition 6.9 is in the flow-rule and the enthalpy inequality *weaker* than its penalised counterpart in Definition 6.2. As far as the flow-rule is concerned, we can recover an equivalent of (5.23) from (6.41) if the *mechanic energy equality*

$$\int_\Omega \phi_1 \bullet \nu(T)\,\mathrm{d}x - \int_\Omega \phi_1 \bullet \nu_0\,\mathrm{d}x = \int_0^T \langle\!\langle \mathfrak{s}, \dot\lambda \rangle\!\rangle\,\mathrm{d}t,$$

could be shown for any $\mathfrak{s}$ satisfying (6.42) [16] – this can be done if λ and ν are smooth. Indeed, if the vector (ν, λ) belonged to some $W^{1,2}([0,T],\mathcal{B})$, with $\mathcal{B}$ such that its dual is a separable Banach space, the mechanic energy equality is readily got by exploiting a variant of the chain rule for non-smooth functions (Visintin, 1996, Proposition 4.11)[17] for the function $F(\nu(t),\lambda(t)) = \int_\Omega \phi_1 \bullet \nu(t) + \delta_{\{v=0\}}(\lambda(t) - L \bullet \nu(t))\,\mathrm{d}x + \delta_{\mathcal{Y}^p(\Omega;\mathbb{R}^{d\times d})}(\nu(t))$ with its sub-differential ($U(t)$ in Theorem 6.11) $(0,\mathfrak{s})$. Note that $0 \in \partial_\nu F(\nu(t),\lambda(t))$ due to the fact that ν solves (6.40).

As far as the enthalpy inequality is concerned, we demand an *enthalpy inequality* to be satisfied together with the *total energy balance* – this is inspired by the notion of so-called *entropy solutions* well known e.g. in the context of the Navier-Stokes-Fourier system (see e.g. (Feireisl and Novotný, 2009)). Again, if the *mechanical energy equality* is satisfied and if (w,λ) are smooth we can recover the equality (6.43) . [18]

[16] Note that to recover (5.23), we just need to plug the mechanic energy equality into (6.41).

[17] For the readers convenience, we re-state the Proposition here

Proposition 6.11 ((Visintin, 1996, Proposition 4.11)). *Assume that $F : \mathcal{B} \to \mathbb{R} \cup \{+\infty\}$, where $\mathcal{B}$ is such that its dual is a separable Banach space, is lower-semicontinuous and convex. Further, let $u \in W^{1,2}([0,T],\mathcal{B})$ and let $U \in L^2([0,T],\mathcal{B}')$ be such that*

$$U(t) \in \partial F(u(t)) \qquad \text{for a.a. } t \in [0,T].$$

Then

$$\frac{\mathrm{d}}{\mathrm{d}t} F(u(t)) = \langle U(t), \dot u(t)\rangle \qquad \text{for a.a. } t \in [0,T].$$

[18] If (w,λ) are smooth, we recover from (6.43) the following strong system

$$\dot w - \mathrm{div}(\mathcal{K}(\lambda,w)\nabla w) \geq \delta_S^*(\dot\lambda) + \alpha|\dot\lambda|^q + \Theta(w)\dot\lambda \qquad \text{in } Q, \tag{6.45}$$

$$\big(\mathcal{K}(\lambda,w)\nabla w\big)\cdot n + b\Theta(w) \geq b\theta_{\mathrm{ext}} \qquad \text{on } \Sigma. \tag{6.46}$$

Indeed, to get (6.45) we use the divergence theorem as well by parts integration in (6.43) and choose ζ such that $\mathrm{supp}\zeta(t) \subset \mathrm{int}(\Omega)$ for all $t \in [0,T]$; this yields

$$\int_Q \Big(\dot w - \mathrm{div}(\mathcal{K}(\lambda,w)\nabla w) \geq \delta_S^*(\dot\lambda) + \alpha|\dot\lambda|^q\Big)\zeta\,\mathrm{d}x\,\mathrm{d}t \geq 0,$$

which, since $\dot w - \mathrm{div}(\mathcal{K}(\lambda,w)\nabla w) \geq \delta_S^*(\dot\lambda) + \alpha|\dot\lambda|^q$ is smooth, can be fulfilled *if and only if* (6.45) holds. For the boundary condition we proceed anallogically; only we chose $\zeta = 0$ on $\Omega_\beta \subset \mathrm{int}(\Omega)$ such that $|\Omega \setminus \Omega_\beta| \leq \beta$ and pass with $\beta \to 0$.

Now, if the inequality in (6.45) was strict on some set $\mathcal{A} \subset Q$ of positive measure, this would give that

$$\int_Q \dot w - \mathrm{div}(\mathcal{K}(\lambda,w)\nabla w)\,\mathrm{d}x\,\mathrm{d}t > \int_Q \delta_S^*(\dot\lambda) + \alpha|\dot\lambda|^q + \Theta(w)\dot\lambda\,\mathrm{d}x\,\mathrm{d}t,$$

and, owing to the boundary condition, we would get that

$$\int_\Omega w(T)\ \mathrm{d}x + \int_\Sigma b\Theta(w)\ \mathrm{d}S\,\mathrm{d}t - \int_\Omega w_0\ \mathrm{d}x - \int_\Sigma b\theta_{\mathrm{ext}}\ \mathrm{d}S\,\mathrm{d}t > \int_Q \delta_S^*(\dot\lambda) + \alpha|\dot\lambda|^q + \Theta(w)\dot\lambda\,\mathrm{d}x\,\mathrm{d}t.$$

Furthermore, when combining this with the expression

$$\int_Q \delta_S^*(\dot\lambda) + \alpha|\dot\lambda|^q + \big(\Theta(w) - \theta_{\mathrm{tr}}\big)\vec a\cdot\dot\lambda\,\mathrm{d}x\,\mathrm{d}t = -\int_\Omega \phi_1 \bullet \nu(T) - \phi_1 \bullet \nu_0\,\mathrm{d}x,$$

that is obtained from (6.41), provided the mechanic energy equality is satisfied, similarly as in Remark 6.7, gives is a *contradiction to* (6.44).

Remark 6.12 (Defect measures). Let us note that one of the main reasons why we cannot prove indeed an equality in (6.43) is the *lack of strong compactness* of the sequence $\{\dot\lambda_\varkappa\}$ in $L^q(Q;\mathbb{R}^{M+1})$ as $\varkappa\to\infty$; this lack of strong compactness is directly connected to the fact that we *cannot* prove the mechanic energy equality in the limit problem.

However, we could prove equality in the sense of measures, i.e. we could find a measure μ_0, such that $\delta_S^*(\dot\lambda_\varkappa)+\alpha|\dot\lambda_\varkappa|^2 \overset{*}{\rightharpoonup}\mu_0$ in $\mathcal{M}(Q)$

$$\int_Q \mathcal{K}(\lambda,w)\nabla w\cdot\nabla\zeta - w\dot\zeta \,\mathrm{d}x\,\mathrm{d}t + \int_\Sigma b\Theta(w)\zeta\,\mathrm{d}S\,\mathrm{d}t + \int_\Omega w(T)\zeta(T) - \int_\Omega w_0\zeta(0)\,\mathrm{d}x$$
$$= +\int_\Sigma b\theta_{\mathrm{ext}}\zeta\,\mathrm{d}S\,\mathrm{d}t + \int_Q \zeta\,\mathrm{d}\mu + \int_Q \Big(\delta_S^*(\dot\lambda)+\alpha|\dot\lambda|^2 + \big(\Theta(w)-\theta_{\mathrm{tr}}\big)\vec a\cdot\dot\lambda\Big)\zeta\,\mathrm{d}x\,\mathrm{d}t,$$

with

$$\mu = \mu_0 - (\delta_S^*(\dot\lambda)+\alpha|\dot\lambda|^2)\,\mathrm{d}x\,\mathrm{d}t,\ ^{19}$$

where μ is referred to as *defect measure* (cf. e.g. (Feireisl, 2004; Naumann, 2006)), because it measures the difference between the obtained measure and the (rate of) dissipation due to phase transition. As already pointed out in Remark 6.10, if the obtained solutions were smooth the defect measure vanished.

Let us just note that a similar lack of compactness was also observed when passing from adhesive to brittle delamination in thermo-elastic case in (Rossi and Thomas, 2012); there also the concept of having only an enthalpy inequality or employing defect measures had to be used.

Let us now formulate the main theorem of this subsection.

Theorem 6.13. *Let the assumptions (A1), (A3)-(A7) be satisfied and* $\lambda_0 = L\bullet\nu_0$. *Denote for any* $\varkappa>0$ $(\nu_\varkappa,\lambda_\varkappa,w_\varkappa)\in(\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d}))^{[0,T]}\times W^{1,q}([0,T];L^q(\Omega))$ $\times L^1([0,T];W^{1,1}(\Omega))$ *any weak solution to (6.1) obtained in Theorem 6.3 and let* T *be a generic final time. Then there exists a not-relabeled subsequence of* $\varkappa\to\infty$ *such that*

$$\lambda_\varkappa \overset{*}{\rightharpoonup} \lambda \qquad \text{in } L^\infty([0,T];L^q(\Omega,\mathbb{R}^{M+1})) \tag{6.47}$$
$$\bar\lambda_\varkappa(t) \rightharpoonup \lambda(t) \qquad \forall t\in[0,T] \text{ in } L^q(\Omega;\mathbb{R}^{M+1}), \tag{6.48}$$
$$\dot\lambda_\varkappa \rightharpoonup \dot\lambda \qquad \text{in } L^q(Q;\mathbb{R}^{M+1}), \tag{6.49}$$
$$w_\varkappa \rightharpoonup w \qquad L^r([0,T];W^{1,r}(\Omega)),\ r<\tfrac{d+2}{d+1} \text{ and } w_\varkappa\to w \text{ in } L^1(Q), \tag{6.50}$$

Moreover, for each $t\in[0,T]$ *there exists a subsequence* $\varkappa_{k(t)}$ *such that*

$$\bar\nu_{\varkappa_{k(t)}}(t) \overset{*}{\rightharpoonup} \nu(t) \quad \text{in } L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d})). \tag{6.51}$$

Every (ν,λ,w) *obtained in this way is then a weak solution of (6.38) in the sense of Definition 6.9.*

Proof. [20] For clarity, let us divide the proof into several steps.

Step 1: A-priori estimates, selection of subsequences:
First of all, recall that we established, already in Theorem 6.3, that $(\nu_\varkappa,\lambda_\varkappa,w_\varkappa)$ satisfy the bounds (6.5) - (6.10).

[19] By "$\mathrm{d}x\,\mathrm{d}t$" we abbreviate the Lebesgue measure on $\Omega\times[0,T]$.

[20] We give here a detailed proof in full-length, however a heuristic sketch of some ideas of this proof is given already in (Benešová, Kružík and Roubíček, 2012).

Let us now even (slightly) enhance (6.6) by exploiting the weak flow-rule for the penalized system (5.23); let us choose $v = \dot\lambda - \tilde v$ with some $\tilde v \in L^2(Q;\mathbb{R}^{M+1})$ such that $\|\tilde v\|_{L^2(Q;\mathbb{R}^{M+1})} = 1$ to get[21]

$$\begin{aligned}\int_0^T \varkappa\langle\!\langle \lambda_\varkappa - L\bullet\nu_\varkappa, \tilde v\rangle\!\rangle\,\mathrm{d}t &\le \int_Q \big(\Theta(w_\varkappa)-\theta_{\mathrm{tr}}\big)\vec a\cdot(-\tilde v)+\rho_2(\dot\lambda_\varkappa-\tilde v)-\rho_2(\dot\lambda_\varkappa)\,\mathrm{d}x\,\mathrm{d}t.\\ &\le \int_Q \big|\Theta(w_\varkappa)-\theta_{\mathrm{tr}}\big|\,|\vec a|\,|\tilde v| + |\rho_2(\dot\lambda_\varkappa)| + |\rho_2(\dot\lambda_\varkappa-\tilde v)|\,\mathrm{d}x\,\mathrm{d}t\\ &\le C\int_Q |w_\varkappa| + |\dot\lambda_\varkappa|^2 + |\tilde v|^2\,\mathrm{d}x\,\mathrm{d}t\end{aligned}$$

where the inequality on the last line is got by Young's inequalities similarly as in e.g. *Step 1* of the proof Lemma 5.10. Further, we realize that the last line is even bounded by a constant *independent of* $\varkappa$ through (6.8) and (6.7). Therefore, $\int_0^T \varkappa\langle\!\langle \lambda_\varkappa - L\bullet\nu_\varkappa, \tilde v\rangle\!\rangle\,\mathrm{d}t \le C$; repeating the same procedure with $v = \dot\lambda_\varkappa + \tilde v$ gives that $-\int_0^T \varkappa\langle\!\langle \lambda_\varkappa - L\bullet\nu_\varkappa, \tilde v\rangle\!\rangle\,\mathrm{d}t \le C$ and thus

$$\int_0^T \varkappa\Big|\langle\!\langle \lambda_\varkappa - L\bullet\nu_\varkappa, \tilde v\rangle\!\rangle\Big|\,\mathrm{d}t \le C, \tag{6.52}$$

for any $\tilde v \in L^2(Q;\mathbb{R}^{M+1})$ such that $\|v\|_{L^2(Q;\mathbb{R}^{d+1})} \le 1$, i.e.

$$\varkappa\|\lambda_\varkappa - L\bullet\nu_\varkappa\|_{L^2([0,T];H^{-1}(\Omega;\mathbb{R}^{M+1}))} \le C, \tag{6.53}$$

with some C *independent of* $\varkappa$.

Choosing, in (6.52), $\tilde v(x,t) = \Xi(t)\tilde v_{\mathrm{S}}(x)$ with $\Xi(t) \in L^\infty([0,T])$ such that $|\Xi(t)| \le 1$ for a.a. $t \in [0,T]$ and $\tilde v_{\mathrm{S}} \in L^2(\Omega;\mathbb{R}^{d+1})$ such that $\|\tilde v_{\mathrm{S}}\|_{L^2(\Omega;\mathbb{R}^{M+1})} \le 1$, leads to $\{|\varkappa\langle\!\langle \lambda_\varkappa(t) - L\bullet\nu_\varkappa(t), \tilde v_{\mathrm{S}}\rangle\!\rangle|\}_{\varkappa>0}$ is bounded for a.a. $t \in [0,T]$. This in turn means that

$$\varkappa\|\lambda_\varkappa(t) - L\bullet\nu_\varkappa(t)\|_{H^{-1}(\Omega;\mathbb{R}^{M+1})} \le C \qquad \text{for a.a. } t \in [0,T]. \tag{6.54}$$

Let us point out that (6.54) indeed improves (6.6) for a.a. $t \in [0,T]$, because, for $q = 2$ and our specific choice of $\mathfrak{Q}$, (6.6) assures only that $\|\lambda_\varkappa(t) - L\bullet\nu_\varkappa(t)\|_{H^{-1}(\Omega;\mathbb{R}^{M+1})}$ scales with the power $\varkappa^{-1/2}$ while (6.54) gives a scaling of the power $\varkappa^{-1}$.

Relying on these a-priori estimates, we choose a subsequence of $\varkappa$ is such that (6.47)-(6.50) hold.[22] Moreover, as in *Step 1* of the proof Proposition 6.5, we employ Helly's selection principle to get

$$w_\varkappa(t) \rightharpoonup w(t) \qquad \text{for all } t \in [0,T] \text{ weakly in } W^{1,r}(\Omega). \tag{6.55}$$

Furthermore, owing to (6.53), we may find $\mathfrak{s} \in L^2([0,T];H^{-1}(\Omega;\mathbb{R}^{M+1}))$ and (if necessary) extract a further subsequence of $\varkappa$'s (not relabeled) such that

$$\varkappa(\lambda_\varkappa - L\bullet\nu_\varkappa) \rightharpoonup \mathfrak{s} \qquad \text{weakly in } L^2([0,T];H^{-1}(\Omega;\mathbb{R}^{M+1})). \tag{6.56}$$

Also, as $\int_\Omega \phi_1\bullet\nu(T)\,\mathrm{d}x + \mathcal{Q}_\varkappa(\lambda_\varkappa(T) - L\bullet\nu_\varkappa(T))$ is , due to (6.5) and (6.6), a *bounded sequence of numbers* we may choose that subsequence of $\varkappa$'s in such a way that

$$\mathcal{E} = \lim_{\varkappa\to\infty}\Big(\int_\Omega \phi_1\bullet\nu(T)\,\mathrm{d}x\mathcal{Q}_\varkappa(\lambda_\varkappa(T) - L\bullet\nu_\varkappa(T)),\Big) \tag{6.57}$$

[21] Note that we already used that $q = 2$ and the specific chosen form of $\mathfrak{Q}$.

[22] Note that we can employ, to this end, the same selection principles as in *Step 3* of the proof Proposition 5.9.

for some $\mathcal{E} \in \mathbb{R}$.

Finally, let us fix some time $t \in [0,T]$ such that the bound in (6.54) holds.[23] Then, based on (6.5), we select a *t-dependent* subsequence of $\varkappa$'s denoted $\varkappa_{k(t)}$ such that

$$\nu_{\varkappa_{k(t)}}(t) \overset{*}{\rightharpoonup} \nu(t) \qquad \text{weakly* in } L^\infty_{\mathrm{w}}(\Omega;\mathcal{M}(\mathbb{R}^{d\times d})), \tag{6.58}$$

with $\nu(t)$ in $\mathcal{Y}^p(\Omega;\mathbb{R}^{d\times d})$, i.e. we got (6.51). Similarly as in *Step 1* of the proof Proposition 6.5, (6.58) yields that $L\bullet\nu_{\varkappa_{k(t)}}(t) \to L\bullet\nu(t)$ *weakly* in $L^2(\Omega;\mathbb{R}^{M+1})$ and thus *strongly* in $H^{-1}(\Omega;\mathbb{R}^{M+1})$.

Exploiting the strong convergence of $L\bullet\nu_{\varkappa_{k(t)}}(t) \to L\bullet\nu(t)$ and also $\lambda_{\varkappa_{k(t)}}(t) \to \lambda(t)$[24] in $H^{-1}(\Omega;\mathbb{R}^{M+1})$ and the a-priori estimate (6.54) we get that for the limits

$$\lambda(x,t) = L\bullet\nu_x(t) \qquad \text{for a.a. } t\in[0,T], \text{ a.e. on } \Omega.^{25} \tag{6.59}$$

Thus, the limit of $L\bullet\nu_{\varkappa_{k(t)}}(t)$ is, for a given λ obtained above, again determined *uniquely* and hence $L\bullet\nu_\varkappa(t) \rightharpoonup L\bullet\nu(t)$ weakly in $L^2(\Omega;\mathbb{R}^{M+1})$. By the Lebesgue dominated convergence theorem, we even get that $L\bullet\nu_\varkappa \to L\bullet\nu$ *strongly* in $L^2([0,T];H^{-1}(\Omega;\mathbb{R}^{M+1}))$.

Step 2: Limit passage in the minimization principle (6.3)
Let $t\in[0,T]$ be still fixed and chosen such that the bound in (6.54) holds. By means of exploiting the lower semi-continuity of $\int_\Omega \phi_1\bullet\nu\,\mathrm{d}x$, as e.g. already in *Step 1* of the proof Theorem 5.15, one gets that

$$\begin{aligned}\int_\Omega \phi_1\bullet\nu\,\mathrm{d}x &\le \liminf_{\varkappa_{k(t)}\to\infty}\int_\Omega \phi_1\bullet\nu_{\varkappa_{k(t)}}\,\mathrm{d}x\\ &\le \liminf_{\varkappa_{k(t)}\to\infty}\int_\Omega \phi_1\bullet\nu_{\varkappa_{k(t)}}\,\mathrm{d}x+\frac{\varkappa_{k(t)}}{2}\|\lambda_{\varkappa_{k(t)}}-L\bullet\nu_{\varkappa_{k(t)}}\|^2_{H^{-1}(\Omega;\mathbb{R}^{M+1})}.\end{aligned} \tag{6.60}$$

Further, we have realize that, *due to the convexity*, any solution of (6.3) $\nu_\varkappa$, solves also the following problem (for the fixed t)[26]

$$\left.\begin{array}{ll}\text{minimize} & \displaystyle\int_\Omega \phi_1\bullet\nu\,\mathrm{d}x+\varkappa\big\langle\!\big\langle \lambda_\varkappa(t)-L\bullet\nu_\varkappa, \lambda_\varkappa(t)-L\bullet\nu\big\rangle\!\big\rangle\\ \text{subject to} & \nu\in\mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d}) \text{ and } \nu_\varkappa \text{ solution to (6.3).}\end{array}\right\} \tag{6.61}$$

Now we return to (6.60) (and use that $\varkappa_{k(t)}/2 \le \varkappa_{k(t)}$) but, instead of exploiting that $\nu_{\varkappa_{k(t)}}$ solves (6.3), we use that it solves (6.61) and get

$$\begin{aligned}&\liminf_{\varkappa_{k(t)}\to\infty}\int_\Omega \phi\bullet\nu_{\varkappa_{k(t)}}\,\mathrm{d}x+\frac{\varkappa_{k(t)}}{2}\|\lambda_{\varkappa_{k(t)}}-L\bullet\nu_{\varkappa_{k(t)}}\|^2_{H^{-1}(\Omega;\mathbb{R}^{M+1})}\\ &= \liminf_{\varkappa_{k(t)}\to\infty}\int_\Omega \phi\bullet\nu_{\varkappa_{k(t)}}\,\mathrm{d}x+\varkappa_{k(t)}\big\langle\!\big\langle \lambda_{\varkappa_{k(t)}}-L\bullet\nu_{\varkappa_{k(t)}}, \lambda_{\varkappa_{k(t)}}-L\bullet\nu_{\varkappa_{k(t)}}\big\rangle\!\big\rangle\\ &\le \liminf_{\varkappa_{k(t)}\to\infty}\int_\Omega \phi\bullet\hat\nu\,\mathrm{d}x+\varkappa_{k(t)}\big\langle\!\big\langle \lambda_{\varkappa_{k(t)}}-L\bullet\nu_{\varkappa_{k(t)}}, \lambda_{\varkappa_{k(t)}}-L\bullet\hat\nu\big\rangle\!\big\rangle\end{aligned}$$

[23] Recall, that the mentioned bound holds for a.a. $t\in[0,T]$.

[24] This is a direct consequence of (6.47) combined with (6.2) and the compact embedding $L^2(\Omega;\mathbb{R}^{M+1}) \overset{\mathrm{c}}{\hookrightarrow} H^{-1}(\Omega;\mathbb{R}^{M+1})$.

[25] In particular, we also got that $L\bullet\nu$ is measurable.

[26] Note that exploiting *just* (6.3) on the right hand side of (6.60) is *not sufficient*. Indeed, if we estimated the right-hand side of (6.60) as $\liminf_{\varkappa_{k(t)}\to\infty}\int_\Omega \phi_1\bullet\hat\nu\,\mathrm{d}x+\frac{\varkappa_{k(t)}}{2}\|\lambda_{\varkappa_{k(t)}}-L\bullet\hat\nu\|^2_{H^{-1}(\Omega;\mathbb{R}^{M+1})}$ with some arbitrary $\hat\nu\in\mathcal{Y}^p(\Omega;\mathbb{R}^{d\times d})$(thanks to (6.3)), it would seem logical to take $\hat\nu$ such that $\lambda(t) = L\bullet\hat\nu$; then, the penalization term on the right-hand side would become $\varkappa_{k(t)}\|\lambda_{\varkappa_{k(t)}}(t)-\lambda(t)\|^2_{H^{-1}(\Omega;\mathbb{R}^{d+1})}$. However, although we know that $\|\lambda_{\varkappa_{k(t)}}(t)-\lambda(t)\|^2_{H^{-1}(\Omega;\mathbb{R}^{d+1})}$ converges to 0 as $\varkappa_{k(t)}\to\infty$, this no longer needs to hold if the term is multiplied by $\varkappa_{k(t)}$.

for all $\hat{\nu} \in \mathscr{Y}^p(\Omega;\mathbb{R}^{d\times d})$ such that $\lambda = L \bullet \hat{\nu}$. Now we exploit our special choice of t for which we know that $\varkappa_{k(t)}\|\lambda_{\varkappa_{k(t)}}(t) - L\bullet\nu_{\varkappa_{k(t)}}(t)\|_{H^{-1}(\Omega;\mathbb{R}^{d+1})}$ is bounded and $\lambda_{\varkappa_{k(t)}}(t) \to \lambda(t)$ strongly in $H^{-1}(\Omega;\mathbb{R}^{d+1})$, which makes the penalization term vanish. Hence we establish the converged minimization principle (6.40).

Let us note that the above procedures also gives that $\mathcal{E} = \int_\Omega \phi_1 \bullet \nu(T)\,\mathrm{d}x$, similarly as we got (5.96) in *Step 2* of the proof Theorem 5.12.[27]

Step 3: Reformulating the flow-rule and passing to the limit in it
Recall that the penalized flow-rule (5.23)[28] stated that for $v \in L^q(Q;\mathbb{R}^{M+1})$

$$\int_Q (\Theta(w_\varkappa)-\theta_{\mathrm{tr}})\vec{a}\cdot(v-\dot{\lambda}_\varkappa)+\rho_q(v)\,\mathrm{d}x\,\mathrm{d}t + \int_0^T \big\langle\!\big\langle \mathfrak{s}_\varkappa, v-\dot{\lambda}_\varkappa\big\rangle\!\big\rangle\,\mathrm{d}t \geq \int_Q \rho_q(\dot{\lambda}_\varkappa)\,\mathrm{d}x\,\mathrm{d}t,$$

where we denoted $\mathfrak{s}_\varkappa = \varkappa(\lambda_\varkappa - L\bullet\nu_\varkappa)$. Furthermore, since the functional $\mathcal{Q}_\varkappa(\cdot)$ is *convex*, $\mathfrak{s}_\varkappa$ has to fulfill

$$\int_0^T \big\langle\!\big\langle \mathfrak{s}_\varkappa, \mathfrak{v}_\varkappa - \lambda_\varkappa\big\rangle\!\big\rangle\,\mathrm{d}t \leq \int_0^T \mathcal{Q}_\varkappa(\mathfrak{v}_\varkappa - L\bullet\nu_\varkappa) - \mathcal{Q}_\varkappa(\lambda_\varkappa - L\bullet\nu_\varkappa)\,\mathrm{d}t, \tag{6.62}$$

for all $\mathfrak{v}_\varkappa \in L^2(Q;\mathbb{R}^{M+1})$. Even, demanding (6.62) is *equivalent* to saying that $\mathfrak{s}_\varkappa = \varkappa(\lambda_\varkappa - L\bullet\nu_\varkappa)$.

Further, let us plug (6.36) with $\lambda_0 = L\bullet\nu_0$ into (5.23) to obtain

$$\begin{aligned}\int_Q (\Theta(w_\varkappa)-\theta_{\mathrm{tr}})\vec{a}\cdot(v-\dot{\lambda}_\varkappa)+\rho_q(v)\,\mathrm{d}x\,\mathrm{d}t + \int_0^T \big\langle\!\big\langle \mathfrak{s}_\varkappa, v\big\rangle\!\big\rangle\,\mathrm{d}t - \mathcal{Q}_\varkappa(\lambda_\varkappa(T)-L\bullet\nu_\varkappa(T)) - \\ \int_\Omega \phi_1\bullet\nu_\varkappa(T) - \phi_1\bullet\nu_0\,\mathrm{d}x \geq \int_Q \rho_q(\dot{\lambda}_\varkappa)\,\mathrm{d}x\,\mathrm{d}t.\end{aligned} \tag{6.63}$$

Applying $\liminf_{\varkappa\to\infty}$ on the right-hand side of (6.63) as well as $\lim_{\varkappa\to\infty}$ on the left-hand side of (6.63) and using (6.56) together with the same ideas as in *Step 4* of the proof Proposition 5.9 leads to:

$$\begin{aligned}\int_Q \rho_q(\dot{\lambda})\,\mathrm{d}x\,\mathrm{d}t &\leq \liminf_{\varkappa\to\infty}\int_Q \rho_q(\dot{\lambda}_\varkappa)\,\mathrm{d}x\,\mathrm{d}t \\ &\leq \liminf_{\varkappa\to\infty}\Big(\int_Q (\Theta(w_\varkappa)-\theta_{\mathrm{tr}})\vec{a}\cdot(v-\dot{\lambda}_\varkappa)+\rho_q(v)\,\mathrm{d}x\,\mathrm{d}t + \int_0^T \big\langle\!\big\langle \mathfrak{s}_\varkappa, v\big\rangle\!\big\rangle\,\mathrm{d}t \\ &\qquad - \mathcal{Q}_\varkappa(\lambda_\varkappa(T)-L\bullet\nu_\varkappa(T)) - \int_\Omega \phi_1\bullet\nu_\varkappa(T)-\phi_1\bullet\nu_0\,\mathrm{d}x\Big) \\ &= \int_Q (\Theta(w)-\theta_{\mathrm{tr}})\vec{a}\cdot(v-\dot{\lambda})+\rho_q(v)\,\mathrm{d}x\,\mathrm{d}t + \int_0^T \big\langle\!\big\langle \mathfrak{s}, v\big\rangle\!\big\rangle\,\mathrm{d}t - \mathcal{E} + \int_\Omega \phi_1\bullet\nu_0\,\mathrm{d}x \\ &= \int_Q (\Theta(w)-\theta_{\mathrm{tr}})\vec{a}\cdot(v-\dot{\lambda})+\rho_q(v)\,\mathrm{d}x\,\mathrm{d}t + \int_0^T \big\langle\!\big\langle \mathfrak{s}, v\big\rangle\!\big\rangle\,\mathrm{d}t \\ &\qquad - \int_\Omega \phi_1\bullet\nu(T)-\phi_1\bullet\nu_0\,\mathrm{d}x,\end{aligned} \tag{6.64}$$

i.e. we passed to the limit in the *reformulated flow-rule* and have obtained 6.41.

Further, let us pass to the limit in (6.62). To this end, we realize that $\mathcal{Q}_\varkappa(\lambda_\varkappa - L\bullet\nu_\varkappa) \geq 0$ and thus, from (6.62),

$$\int_0^T \big\langle\!\big\langle \mathfrak{s}_\varkappa, \mathfrak{v}_\varkappa - \lambda_\varkappa\big\rangle\!\big\rangle\,\mathrm{d}t \leq \int_0^T \mathcal{Q}_\varkappa(\mathfrak{v}_\varkappa - L\bullet\nu_\varkappa) - \mathcal{Q}_\varkappa(\lambda_\varkappa - L\bullet\nu_\varkappa)\,\mathrm{d}t \leq \int_0^T \mathcal{Q}_\varkappa(\mathfrak{v}_\varkappa - L\bullet\nu_\varkappa)\,\mathrm{d}t.$$

[27] Since T is a *generic* final time, we may chose it in such a manner that (6.53) holds.
[28] Here already rewritten using our specific form of $\mathcal{Q}_\varkappa$ and $q = 2$.

Let us choose $\mathfrak{v}_\varkappa = L\bullet\nu_\varkappa + \mathfrak{v} - L\bullet\nu$ with any $\mathfrak{v} \in L^{Q;\mathbb{R}^{M+1}}$ such that $\mathfrak{v}(x,t) = L\bullet\nu_x(t)$ for a.a. $t\in[0,T]$, a.e on Ω. Then $\mathfrak{v}_\varkappa \to \mathfrak{v}$ *strongly* in $L^2([0,T];H^{-1}(\Omega;\mathbb{R}^{M+1}))$ thanks to the ideas exposed in the last paragraph of *Step 1*. Furthermore, with this choice, $\int_0^T \mathcal{Q}_\varkappa(\mathfrak{v}_\varkappa - L\bullet\nu_\varkappa)\,\mathrm{d}t = 0$ identically and thus applying $\lim_{\varkappa\to\infty}$ gives

$$\int_0^T \big\langle\!\big\langle \mathfrak{s}_\varkappa, \mathfrak{v}_\varkappa - \lambda_\varkappa \big\rangle\!\big\rangle\,\mathrm{d}t \le 0 \qquad \text{for all } \mathfrak{v}\in L^2(Q;\mathbb{R}^{M+1}) \text{ such that } \mathfrak{v}(x,t) = L\bullet\nu_x(t) \text{ for a.a. } t\in[0,T], \text{ a.e on } \Omega,$$

i.e. we got (6.42).

Step 4: Total energy equality
In this step we deduce that the *total energy* is also conserved in the case when the limit $\varkappa\to\infty$ has is been applied.

To this end, we exploit that we know, from *Step 1* and *Step 2*, that $\mathcal{Q}_\varkappa(\lambda_\varkappa - L\bullet\nu_\varkappa) + \int_\Omega \phi_1\bullet\nu_\varkappa(T) \to \int_\Omega \phi_1\bullet\nu(T)$ and the assumtion that $\lambda_0 = L\bullet\nu_0$. Thus, the right-hand side of (6.37) converges to the right-hand side of (6.44) if $\varkappa\to\infty$.

On the left-hand side, we exploit the Aubin-Lions theorem and interpolation as in *Step 7* of the proof Proposition 5.9 to get that, for any $\delta>0$ small, the traces of $w_\varkappa$ converge strongly in $L^{(d+2)/(d+1)-\delta}([0,T];L^{(d^2+d-2)/(d^2-2)-\delta}(\Gamma))$ to the traces of w; thus, $\int_\Sigma b\Theta(w_\varkappa)\,\mathrm{d}S\,\mathrm{d}t \to \int_\Sigma b\Theta(w)\,\mathrm{d}S\,\mathrm{d}t$. Next, we employ (6.55) to get that $\int_\Omega w_\varkappa(T)\,\mathrm{d}x \to \int_\Omega w(T)\,\mathrm{d}x$ and, finally, (6.49) to get that $\int_Q \theta_{\rm tr}\vec{a}\cdot\dot\lambda_\varkappa\,\mathrm{d}x\,\mathrm{d}t \to \int_Q \theta_{\rm tr}\vec{a}\cdot\dot\lambda_\varkappa\,\mathrm{d}x\,\mathrm{d}t$ as $\varkappa\to\infty$. Hence, also the left-hand side of (6.37) converges to the left-hand side of (6.44).

Step 5: Enthalpy inequality
At last, we pass to the limit $\varkappa\to\infty$ in (6.4) to obtain (6.43). To this goal, we only need to show that

$$\int_Q (\delta_S^*(\dot\lambda) + \alpha|\dot\lambda|^2)\zeta\,\mathrm{d}x\,\mathrm{d}t \le \liminf_{\varkappa\to\infty}\int_Q (\delta_S^*(\dot\lambda_\varkappa) + \alpha|\dot\lambda_\varkappa|^2)\zeta\,\mathrm{d}x\,\mathrm{d}t,$$

for any $\zeta\in C^1(\bar Q)$ such that $\zeta\ge 0$; all other terms in (6.4) can be handled analogously to *Step 4*. Let us take any smooth ζ and approximate it by piecewise constant functions ζ_k such that

$$\zeta_k = A_i \qquad \text{on } Q_i,$$

with Q_i pairwise disjoint and $Q=\bigcup_i Q_i$; then $\zeta_k\to\zeta$ strongly (and also independently of $\varkappa$); $A_i\ge 0$ since $\zeta\ge 0$. Then

$$\int_Q (\delta_S^*(\dot\lambda_\varkappa) + \alpha|\dot\lambda_\varkappa|^2)\zeta_k\,\mathrm{d}x\,\mathrm{d}t = \sum_i A_i\int_{Q_i}(\delta_S^*(\dot\lambda_\varkappa) + \alpha|\dot\lambda_\varkappa|^2)\,\mathrm{d}x\,\mathrm{d}t.$$

Exploiting now weak lower semicontinuity due to (6.49) gives

$$\begin{aligned}\sum_i A_i\int_{Q_i}(\delta_S^*(\dot\lambda) + \alpha|\dot\lambda|^2)\,\mathrm{d}x\,\mathrm{d}t &\le \sum_i A_i \liminf_{\varkappa\to\infty}\int_{Q_i}(\delta_S^*(\dot\lambda_\varkappa) + \alpha|\dot\lambda_\varkappa|^2)\,\mathrm{d}x\,\mathrm{d}t\\ &\le \liminf_{\varkappa\to\infty}\Big(\sum_i A_i\int_{Q_i}(\delta_S^*(\dot\lambda_\varkappa) + \alpha|\dot\lambda_\varkappa|^2)\,\mathrm{d}x\,\mathrm{d}t\Big);\end{aligned}$$

and passing with $k\to\infty$ gives the claim. □

Chapter 7

Numerical implementation of thermally coupled model

Providing a numerical implementation of the proposed models is important in order to demonstrate quantitatively or at least qualitatively their predictive capabilities and, if possible, compare the results to experiments or theoretical predictions. Later, if the numerical implementation of the model gives satisfactory results, the implementation can be used to predict responses of the specimen in situations in which an experimental study would be expensive or even impossible.

Within this chapter, we provide details on numerical implementation of thermo-mechanically coupled model devised in Chapter 5 based on the existence proof via time-discretization presented in Section 5.5. To this end, we present details on the used spatial discretization and implementation of the discrete problem in Section 7.1; herein we us ideas from the works (Arndt et al., 2006; Kružík, 1998; Kružík et al., 2005; Roubíček et al., 2007) and others.[1] In Section 7.2, we outline the most important difficulties connected with the numerical solution of the governing equations (5.17) and propose some strategies to improve computations. Let us note that Section 7.2 is based on results already published in (Benešová, 2011*a*).

Finally, in Section 7.3, we present results of a calculation, performed within the numerical implementation presented here, for the double-well problem; these calculations were not published before. We chose the double well problem because, in spite of its simplicity, one can demonstrate a lot of the important predictive capabilities of the model on it. Nevertheless, a huge drawback of the double well-problem is that it cannot be related to any SMA material; performing calculations with relevant physical data thus remains as a challenge for the future.

Although the importance of fast and robust and also easy-to-use numerical implementations is undeniable, within this thesis we focused rather on model development and the study of existence of solutions to it. This justifies the restriction to the double well problem or very simple meshing. Nevertheless, due to the necessity to properly approximate gradient Young measures, the non-convexity and the non-smoothness of the problem, obtaining even the presented results is lengthy and requires care, e.g. in the choice of initial conditions, efficient minimization algorithms, and also a lot of programming work.

[1] The numerical implementation presented within this chapter has been "from scratch" programmed within this thesis building upon the results from (Benešová, 2008); however, several external routines are exploited e.g. for solving algebraic systems and some minimization problems. While the obtained code is then easily adjustable at any point, in future it would be advantageous to connect the obtained code with freely and/or commercially available programs to allow for e.g. automatic meshing and mesh refinement, optimized storage, automatic differentiation etc.

7.1 Details on discretization and implementation

Clearly, in order to devise a numerical implementation of thermally coupled model (5.17) one has to introduce a discretization of the time-interval $[0,T]$ and also a spatial discretization of the reference domain Ω.

As far as the time discretization is concerned, we follow Section 5.5 and introduce a uniform partition $0 = t_0 \leq t_1 \leq t_2 \dots t_N = T$ of the interval $[0,T]$ such that $(t_{i+1} - t_i) = \tau$ for $i = 1 \dots N$ and some τ prescribed by the user of the numerical routine.

For the discretization of the reference domain Ω, we assume that Ω is a *polyhedral domain*[2] $\subset \mathbb{R}^3$; we then introduce a triangulation τ_h of Ω formed by a collection of tetrahedra that we denote $\{K_i\}_{i=1}^{P(h)}$.[3]

7.1.1 Discretization of the relevant function spaces

When devising the time-discrete equivalent of (5.17) in (5.103), we introduced the time-discrete vector of volume fractions, at time-level k, $\lambda_\tau^k \in L^{2q}(\Omega;\mathbb{R}^{M+1})$, the discrete enthalpy $w_\tau^k \in W^{1,2}(\Omega)$ and the discrete deformation/microstructure $(y_\tau^k, \nu_\tau^k) \in W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^3) \times \mathscr{G}_{\Gamma_D}(\Omega;\mathbb{R}^{3\times 3})$.[4] We shall approximate the functions spaces in which these state variables lie by spaces of piecewise affine or piecewise constant functions; in particular, we introduce $\lambda_{\tau,h}^k$ as an approximation of λ_τ^k satisfying

$$\lambda_{\tau,h}^k \in \Lambda_{\tau,h} = \Big\{ \tilde{\lambda} \in L^\infty(\Omega;\mathbb{R}^{M+1});\ \text{such that } \tilde{\lambda}_{|K_i} \text{ is constant } \forall i = 1 \dots P(h) \Big\}, \quad (7.1)$$

the approximative enthalpy $w_{\tau,h}^k$ is taken from the space

$$w_{\tau,h}^k \in \mathcal{W}_{\tau,h} = \Big\{ \tilde{w} \in C(\bar{\Omega});\ \text{such that } \tilde{w}_{|K_i} \text{ is affine } \forall i = 1 \dots P(h) \Big\}, \quad (7.2)$$

and, furthermore, the discrete deformation $y_{\tau,h}^k$ is also assumed to be piecewise affine, however satisfying the prescribed Dirichlet boundary condition, i.e.

$$y_{\tau,h}^k \in Y_{\tau,h} = \Big\{ u \in C(\bar{\Omega};\mathbb{R}^3),\ \text{such that } u_{|K_i} \text{ is affine, } \forall k = 1 \dots M \\ \text{and } u(x_B) = x_B \text{ for all vertices } x_B \text{ for which } \Gamma_D \cap x_B \neq \emptyset \Big\}. \quad (7.3)$$

Thus, it remains to devise a discretization of the space of Young measure $\mathscr{G}_{\Gamma_D}(\Omega;\mathbb{R}^{3\times 3})$. For this, we exploit the ideas of Section 2.3 and approximate the gradient Young measures by laminates of finite order ℓ, i.e.

$$\nu_{\tau,h}^k \in \mathscr{G}_{\tau,h}^\ell = \Big\{ \tilde{\nu} \in L^\infty(\Omega;\mathcal{M}(\mathbb{R}^{3\times 3})) \text{ such that } \tilde{\nu}_{|K_i} = \sum_{i=1}^{2\ell} \lambda_i \delta_{F_i} \text{with } (\lambda_i, F_i) \\ \text{satisfying the } \ell\text{-th order laminate condition from Definition 2.15.} \Big\} \quad (7.4)$$

In the presented implementation, the lamination order ℓ can be chosen arbitrarily; in practise, however, second order laminates are used at most.[5]

[2] If Ω was not polyhedral, we had to approximate it by a polyhedral domain. Clearly, one can approximate any smooth domain by a polyhedral one as precisely as demanded. Also note that, for implementation we consider only the case $d = 3$.

[3] Though generally we could assume that the triangulation varies from time-step to time-step, in some cases, as when investigating backtracking algorithms as in Section 7.2, we shall need it to be fixed for the whole evolution. Thus, for simplicity, we shall adopt the assumption of non-varying triangulation during evolution everywhere within this chapter.

[4] Recall that for implementation we limit ourselves to the case $d = 3$.

[5] This is due to the fact that laminates observed in nature are mostly of the second order (see e.g. (Bhattacharya, 2003) or (Otsuka and Ren, 2005)).

Even though, as we stressed in Chapter 2, the *set of laminates does not coincide with the set of gradient Young measures* such an approximation is still justified. Namely, it can be shown that, with mesh refinement, for any $\nu \in \mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^{3\times 3})$, a sequence of $\nu_h \in \mathscr{G}^\ell_{\tau,h}$ can be found such that $\nu_h \overset{*}{\rightharpoonup} \nu$ in $L^\infty(\Omega;\mathcal{M}(\mathbb{R}^{3\times 3}))$ (Benešová, 2008).

Note that we did not impose any boundary conditions within the space $\mathscr{G}^\ell_{\tau,h}$; we shall inforce them by requiring that

$$\nabla y^k_{\tau,h} = \mathrm{id} \bullet \nu^k_{\tau,h}, \tag{7.5}$$

everywhere on Ω. This condition, actually, needs only to be satisfied element-wise since both, $\nabla y^k_{\tau,h}$ and $\nu^k_{\tau,h}$, are piecewise constant.

Remark 7.1 (Compatibility of the spatial discretization). Note that the space $Y_{\tau,h}$ is *compatible* with $\mathscr{G}^\ell_{\tau,h}$ in the sense that $Y_{\tau,h}$ contains piecewise affine functions; hence the gradients of functions in $Y_{k,h}$ are piecewise constant – and so are elements from $\mathscr{G}^\ell_{\tau,h}$. Thus it is *possible* to satisfy (7.5) everywhere on Ω. Similarly, $\Lambda_{\tau,h}$ contains piece-wise constant functions, which will allow us to demand $\lambda^k_{\tau,h} \approx L \bullet \nu^k_{\tau,h}$.

Remark 7.2 (Degrees of freedom). At first glance, introducing a laminate of the ℓ^{th} order and the deformation on one tetrahedron requires to introduce, as degrees of freedom, $2{\cdot}\ell$ matrices F_i, $2{\cdot}\ell$ coefficients λ_i and the values of $y^k_{\tau,h}$ in 4 vertices – hence we would have $2\ell \times 9 + 2\ell + 4 \times 3$ degrees of freedom on one element. Yet, this calculations did not take into account that F_i are rank-1 connected, that λ_i sum up to 1 nor that (7.5) has to be satisfied.

In order to meet all constrains on F_i and λ_i, we adopt a recursive tree-like procedure to define the laminate and the deformation through a minimum number of variables, cf. e.g. (Kružík, 1998). Let us illustrate this procedure for a laminate of order one, for order two we refer to Figure 7.1 and higher orders can be constructed analogously. In the case of a laminate of order one, note that the matrices F_1 and F_2, forming the rank-1-partition of the deformation gradient $\nabla y^k_{\tau,h}$, are fully determined by the deformation gradient itself, a weight λ and two vectors $\mathbf{a}$ and $\mathbf{n}$, i.e.[6]

$$\begin{aligned} F_1 &= \nabla y^k_{\tau,h} + (1-\lambda)\mathbf{a}\otimes\mathbf{n},\\ F_2 &= \nabla y^k_{\tau,h} - \lambda\mathbf{a}\otimes\mathbf{n}. \end{aligned}$$

Thus, only $2\ell \times 7 + 4 \times 3$ degrees of freedom per element are needed to specify $y^k_{\tau,h}$ and $\nu^k_{\tau,h}$.

Having introduced the spatial discretization, the fully discrete analog of (5.17) reads, in any time-step t_k, as:

Find the a quadruple $(y^k_{\tau,h}, \nu^k_{\tau,h}, \lambda^k_{\tau,h}, w^k_{\tau,h}) \in Y_{\tau,h} \times \mathscr{G}^\ell_{\tau,h} \times \Lambda_{\tau,h} \times \mathcal{W}_{\tau,h}$ satisfying (7.5) and

1. The **minimization problem for** λ with given $\lambda^{k-1}_{\tau,h}$, $w^{k-1}_{\tau,h}$ and $\nu^{k-1}_{\tau,h}$:

$$\left.\begin{aligned} &\text{Minimize} \quad \mathcal{G}(t_k, y^{k-1}_{\tau,h}, \nu^{k-1}_{\tau,h}, \lambda, \Theta(w^{k-1}_{\tau,h})) + \tau\int_\Omega |\lambda|^{2q} + \rho_q\Big(\frac{\lambda-\lambda^{k-1}_{\tau,h}}{\tau}\Big)\\ &\text{subject to} \quad \lambda \in \Lambda_{\tau,h}. \end{aligned}\right\} \tag{7.6a}$$

   with $\mathcal{G}$ from (5.6).

2. The **minimization problem for** (y,ν) with given $\lambda^k_{\tau,h}$:

$$\left.\begin{aligned} &\text{Minimize} \quad \mathfrak{G}(t_k, y, \nu, \lambda^k_{\tau,h})\\ &\text{subject to} \quad (y,\nu) \in Y_{\tau,h} \times \mathscr{G}^\ell_{\tau,h} \text{ satisfying (7.5).} \end{aligned}\right\} \tag{7.6b}$$

[6] Similar relations hold also for the matrices $F_{12} \dots F_{22}$ following Figure 7.1.

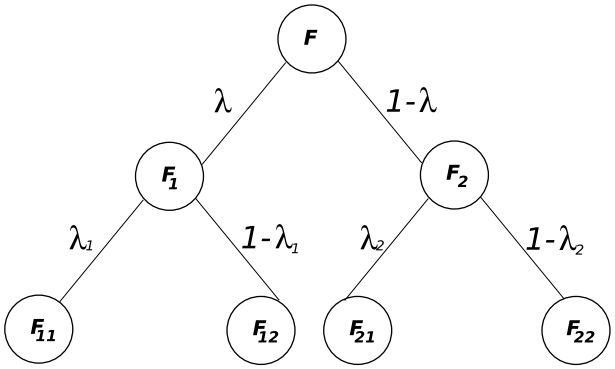


Figure 7.1: The scheme of the rank-1-partition of the deformation in case of a second order laminate; in the figure we denoted $F = \nabla y^k_{\tau,h}$.

with $\mathfrak{G}$ defined in (5.93).

3. The **enthalpy equation**: For all $\varphi \in \mathcal{W}_{\tau,h}$

$$\int_\Omega \Big(\frac{w^k_{\tau,h}-w^{k-1}_{\tau,h}}{\tau}\Big)\varphi + \mathcal{K}(\lambda^k_{\tau,h}, w^k_{\tau,h})\nabla w^k_{\tau,h}\cdot\nabla\varphi \,\mathrm{d}x + \int_\Gamma b^k_{\tau,h}\Theta(w^k_{\tau,h})\varphi \,\mathrm{d}S$$
$$= \int_\Gamma b^k_{\tau,h}\theta^k_{\mathrm{ext},\tau,h}\varphi \,\mathrm{d}S + \int_\Omega \varrho_q\Big(\frac{\lambda^k_{\tau,h}-\lambda^{k-1}_{\tau,h}}{\tau}\Big)\varphi + \Theta(w^k_{\tau,h})\vec{a}\cdot\Big(\frac{\lambda^k_{\tau,h}-\lambda^{k-1}_{\tau,h}}{\tau}\Big)\varphi \,\mathrm{d}x. \quad (7.6c)$$

with $b^k_{\tau,h}$, $\theta^k_{\mathrm{ext},\tau,h}$ piecewise affine approximations of b^k_τ, $\theta^k_{\mathrm{ext},\tau}$, respectively.

Then, the cost functions in (7.6a) and (7.6b) are evaluated using some numerical quadrature[7]; i.e. (7.6a) and (7.6b) actually represent minimization problem of two cost functions $\mathbb{R}^s \to \mathbb{R}$, where s can take values, depending on the number of elements, of several tens to several thousands. The cost function involved in (7.6a) is *convex and non-smooth*, so local search algorithms can be used. The cost function resulting from (7.6b) is, on the other hand, *non-convex* so local methods have the tendency to stay trapped in local minima – it is therefore better to use a *global minimization method*; those, however, are, except for some special cases, only heuristic with no guarantee of convergence (e.g (Kennedy and Eberhart, 1995) for particle swarm optimization); we address this issue more in detail in Section 7.2.

Finally, (7.6c) is solved by introducing a Lagrangean first order basis and applying the standard procedure of the finite element method.

Remark 7.3 (Replacing (7.6a) and (7.6b) by a single minimization problem). For isothermal systems, as presented in Section 4.2, we had only one minimization problem on the discrete level (4.28). This could inspire us to solve instead of (7.6a) and (7.6b) the

[7] As $\mathscr{G}^\ell_{\tau,h}$ and $\Lambda_{\tau,h}$ contain piecewise constant functions, the numerical quadrature of the Helmholtz free energy and the dissipation potential reduces just to a summation of constant values (multiplied by the measure of the respective element) over all elements. For the volume force term, we adopt the simple quadrature

$$\int_\Omega f(t_k,x)y(t_k,x) \approx \sum_{K_i\in\tau_h}\frac{1}{4}\sum_{x_j\in\text{Vertices of } K_i} f(t_k,x_j)y(t_k,x_j);$$

the surface force usually can be treated as in Remark 7.4.

following minimization problem

$$\left.\begin{array}{ll}\text{Minimize} & \mathcal{G}(t_k, y, \nu, \lambda, \Theta(w_{\tau,h}^{k-1})) + \tau\displaystyle\int_\Omega |\lambda|^{2q} + \rho_q\Big(\frac{\lambda-\lambda_{\tau,h}^{k-1}}{\tau}\Big) \\ \text{subject to} & (y,\nu,\lambda) \in Y_{\tau,h} \times \mathscr{G}_{\tau,h}^{\ell} \times \Lambda_{\tau,h},\end{array}\right\} \tag{7.7}$$

i.e. we minimize jointly in (y, ν) and λ. Yet, solving (7.7) is not backed by a convergence analysis conversely to solving (7.6a) and (7.6b) (except for in the convex case). On the other hand, it can be simply adapted to solving the isothermal rate-independent case; hence, in addition to (7.6a) and (7.6b) also (7.7) was implemented in the presented code and it is up to the user to chose the more suitable minimization routine.

Remark 7.4 (Simplifying the numerical quadrature for constant surface forces). Note that solving (7.6b) implies evaluating the surface integral $\int_{\Gamma_N} g(t)\cdot y \,\mathrm{d}S$. This, however, can be avoided if Ω is a prism and g is a constant surface force that acts only the base side of Ω – we denote $\mathbf{n}$ be the unit normal of this side. Then we may rewrite

$$g\cdot y = ((g\otimes \mathbf{n})\mathbf{n})\cdot y,$$

which, by the usage of the divergence theorem, gives

$$\int_{\Gamma_N} g\cdot y \,\mathrm{d}S = \int_\Omega \mathrm{div}\Big(((g\otimes\mathbf{n})\mathbf{n})\cdot y\Big)\,\mathrm{d}x = \int_\Omega (\mathbf{n}\otimes g)\cdot\nabla y \mathrm{d}x.$$

For, $y \in Y_{\tau,h}$ this reduces to

$$\int_{\Gamma_N} g\cdot y \,\mathrm{d}S = \sum_{K_i\in\tau^k} |K_i|(\mathbf{n}\otimes g)\cdot(\nabla y(t_k, K_i)), \tag{7.8}$$

where we denoted $\nabla y(t_k, K_i)$ the value of the deformation gradient on the i-th element as it is constant element-wise. Thus, in this simplified case the numerical quadrature is much easier.

Remark 7.5 (Choice of the Gibbs free energy/dissipation potential in the numerics). As soon as it comes to numerical implementation, a specific form of the Helmholtz free energy and the dissipation potential has to be prescribed. Within this thesis, we follow (Kružík et al., 2005) and assume ϕ_1 given through

$$\phi_1(F) = \min_{i=1\ldots M+1} \psi_m$$

with ψ_m defined through (4.6) with $c_V^m = 0$; in the dissipation potential we choose $\delta_S(\dot\lambda) = r(\dot\lambda)$ with r defined through (4.15).

Finally, we have to prescribe the function L determining the vector of volume fractions. We follow (Kružík et al., 2005; Roubíček et al., 2007) and work with the following form

$$L(F) = \left\{\frac{\mathfrak{d}(|FF^{\mathrm{T}} - U_l U_l^{\mathrm{T}}|)}{\sum_{k=1}^{M+1}\mathfrak{d}(|FF^{\mathrm{T}} - U_k U_k^{\mathrm{T}}|)}\right\}_{l=1}^{M+1}, \tag{7.9}$$

[8]

Further, the function $\mathfrak{d}\in C(\mathbb{R})$ is chosen such that outside a sufficiently small interval $[-\epsilon,\epsilon]$ it is equal to 0, Further, the norm $|\cdot|$ is the Frobenius norm[9] for matrices. Such a definition of the function L ensures, roughly speaking, that as soon as the deformation gradient – or rather the matrices forming its rank-1 decomposition in the sense of a laminate – are near to the well of some variant, volume fractions are assigned to this variant.

[8] Recall, that $U_1 \ldots U_M$ are distortion matrices corresponding to the variants of martensite; U_{M+1} is the distortion matrix of austenite.

[9] Recall that for a matrix $A\in\mathbb{R}^{3\times3}$ the Frobenius norm is $|A| = \sqrt{\sum_{i,j=1}^3 a_{ij}^2}$ where $\{a_{ij}\}_{i,j=1}^3$ are the elements of the matrix A.

7.1.2 Used algorithms and notes on implementation

In this section let us give very brief notes on the code that solves the problem (7.6a)-(7.6c); this code is an extension of the one implemented in (Benešová, 2008) following the ideas if (Kružík, 1998; Roubíček et al., 2007). We also sketch which algorithms have been implemented.

The code has been written in C++ using the concept of object-oriented programming – to describe it, we are hence entitled to introduce only the most important classes of the code.

- The class `CombinedHeatAndDeformationModel` is the main class of the code, that manages all the classes presented below, used for solving (7.6a) - (7.6c): It reads in results from the last computational step (if appropriate), boundary data, material data and sets up the problem by initializing all variables needed for computation. The class is designed in such a way that *only* routines of this class have to be called by the user in the main program – in particular, its routine `SolveTheCombinedSystemAndWriteData` solves (7.6a) - (7.6c) and exports results in VTK-format so that they may be used for visualized in open source programs such as *ParaView* or *MayAvi*. Further, the class provides also routines to solve only (7.6c) or only (7.6a)-(7.6b). Finally, backtracking (cf. Section 7.2) is also handled within this class.

- The class `IsothermalModel` is responsible for solving of (7.6a) - (7.6b), alternatively it can also solve (7.7) which is advantageous when temperature is considered fixed. It includes built-in functions to perform the rank-1-decomposition of the deformation gradient (cf. Remark 7.7), calculate the mechanic energy as well as to minimize it.

- The class `HeatEquation` is responsible for solving the enthalpy equation (7.6c) – hence, it sets up the algebraic equation corresponding to this finite element problem and solves it by exploiting the external routine `dgesv_` from *CLAPACK* (downloadable at `http://www.netlib.org/clapack`).

- The class `Mesh` reads mesh file given to the code; this has to be provided by an external meshing program – unfortunately the code is not able to do any meshing by itself; we use the external package *NetGen* (downloadable at `http://www.hpfem.jku.at/netgen/`).

- The class `Material` stores all information about the current material, namely the distortion matrices of each variant, elastic constants, the transformation entropy and the specific heat capacities. It is able to read in this information from a data file and save it to appropriate variables.

Besides these main classes the code uses also some helping classes for visualization and for handling vectors or matrices.

Remark 7.6 (Privacy in classes). Most of the built-in functions as well as variables of the classes described above are set to be *private*, which disables the user to alter them (for variables) or call them (for functions) in the main program. This is done to assure security as it prevents users from changing accidentally the computation variables during evaluation.

Remark 7.7 (Implementation of laminates). In the implementation of the rank-1 decomposition of the deformation gradient we follow the scheme in Figure 7.1 and (Roubíček et al., 2007) which suggest to use the structure of a binary tree. $\mathfrak{G}(t_k, y^k_{\tau,h}, \nu^k_{\tau,h}, \lambda^k_{\tau,h})$

is then evaluated recursively when using the scheme from Lemma 2.8. This recursive implementation is advantageous, since it allows for usage of laminates of any order – the order of lamination is chosen at setup of the problem. Moreover, it does not matter whether the binary tree used is symmetric or non-symmetric.

Remark 7.8 (Minimization algorithms). An important issue is the choice minimization algorithms for solving (7.6a), (7.6c) or, alternatively, (7.7). Note that this issue is *highly non-trivial* because (7.6a) includes a non-smooth (albeit convex) objective and in (7.6c) (and similarly in (7.7)) a *highly non-convex* objective is subject to minimization. In both cases, the *number of degrees of freedom can reach up to several thousands* even for coarse meshes. So, the minimization problem combines *most of the difficulties in numerical optimization*.

For (7.6a), being convex, *local search algorithms* can be applied, we use an enhanced version of *L-BFSG* (downloadable at `http://www.chokkan.org/software/liblbfgs`) that also includes the *Orthant-Wise Limited-memory Quasi-Newton* algorithm that can be used for minimizing an objective that is the sum of a smooth convex function and the absolute value.

For (7.6b) or (7.7), we use either local methods or stochastic as well as population-based methods; cf. Section 7.2 for details.

7.2 Computation difficulties and optimization

As already indicated, solving (7.6b) or (7.7) is the most difficult task when obtaining numerical solutions to the system (5.17) (for thermally coupled case) of the system (4.18)-(4.19) (for the isothermal case). Originally, in (Benešová, 2008) (and also in previous works as (Kružík, 1998; Kružík et al., 2005; Roubíček et al., 2007)) (7.7) was solved *just* by a gradient descent method, which, due to the strong non-convexities of the involved cost functions, led to satisfactory results only for special loading situations and if special care has been paid to designing initial conditions.

Therefore, already in (Benešová, 2008), some possible strategies were developed to enhance the search for global minima, these have been further extended within the work on this thesis. In this section, hence, let us summarize the developed optimization strategies for the *isothermal case*, i.e. solving "*just*" (7.7), and comment which of them can generalized to thermally coupled case. Let us note that this section is based on (Benešová, 2011*a*), elaborated within the work on this thesis.

7.2.1 Comparing (7.7) to other problems exploiting global optimization, choice of optimization algorithms

Global optimization plays an important role in a number of applications like in curve fitting or the famous travelling salesman problem; so, one could try to exploit some methods proposed in these cases also for the minimization problems considered here. However, when trying to find discrete solutions to (4.18)-(4.19) through solving (7.7), we do not have to solve *just one* minimization problem but rather a sequence of these problems within which the objective slowly changes; hence, the problems falls within the class *global optimization problems in a dynamic environments* with an objective function that experiences a jump at every time-step. Similarly, solving (7.6b) represents a sequence of minimization problems with the cost function changing in a jump-like manner.[10] Even in this special class of optimization problems, a large amount of research

[10] In the isothermal case, the "jump-like character" of the change of the objective function cannot be avoided, since for continuous time the energetic solution satisfies only the stability condition (and the energy equality), which does not pose a global optimization problem anymore. In thermally coupled

has been carried out recently (see e.g. (Blackwell, 2003; Branke, 2002, 2011; Cobb and Grefenstette, 1993; Grefenstette, 1992) and references therein).

Within the class of global optimization problems in dynamic environments, several sub-classes can be distinguished depending on how the cost function changes (Trojanowski and Michalewicz, 1999)[11]. The problems (7.7) as well as (7.6b), that need to be solved here, fall within the category for which changes are *non-random but not predictable*[12].

For an illustration of the complexity of (7.7), it might be helpful to compare (7.7) to a standard benchmark in global optimization in dynamic environments, namely the *Moving-peaks problem*[13]; a pronounced difference, making (7.7) (as well as (7.6b)) more complicated, is the size of the state space. While the moving peaks benchmark supposes that the dimension of the state space is of the order of tens at most, the dimension of $Y_{k,h} \times \mathscr{G}^{\ell}_{\tau,h}$ is typically in the order of hundreds to thousands, depending on the mesh-size. Further, what makes (7.7) (as well as (7.6b)) especially difficult is the "path-dependence" i.e. the dependence of the objective function on the previously found optima. Because of that, the minima of the cost function at time-step k are directly comparable, *only* if all preceding states of these two were the same. Such a situation is not covered by the moving-peaks benchmark nor the problems considered in the references above.

On the other hand, when solving (7.7) or (7.6b) one can assume that the minimizer in time-step k $q^k_{\tau,h} = (y^k_{\tau,h}, \nu^k_{\tau,h}, \lambda^k_{\tau,h}, w^k_{\tau,h})$ will lie in some neighbourhood of the solution from the last step $q^k_{\tau,h} = (y^k_{\tau,h}, \nu^k_{\tau,h}, \lambda^k_{\tau,h}, w^k_{\tau,h})$, in the moving peaks problem, the cost function can change randomly. Yet, this assumption is rather intuitive, because we were not able to prove in-time continuity of weak solutions to (5.17) nor (4.18)-(4.19); thus even large jumps on the discrete setting are, in principle, not excluded.

Even though the minimization problem posed in (7.7) (or (7.6b)) seems to be more complex than standard global optimization problems solved in dynamic environments, it is still useful to study the type of minimization algorithms used in literature. It has been proposed that population-based[14] algorithms, altered in some suitable way during the computation, are especially suitable for this context (see e.g. (Branke, 2002, 2011)).

Thus, we adapted three different minimization routines for solving (7.7) or (7.6b): a *gradient descent* algorithm[15], the *simulated annealing* method[16] that is *stochastic* but

case, even in the continuous case (5.22) represents a global optimization problem, however coupled to other equations.

[11] In (Trojanowski and Michalewicz, 1999) the author distiguishes between random changes, non-random changes that are so complex that they cannot be predicted and predictable changes.

[12] The change of the cost function (7.7) *cannot* be a-priori determined due to the dissipation term, the time-dependence of which is unknown prior to evolution. Similarly, when solving (7.6b) the cost function depends on time also through the prescribed $\lambda^k_{\tau,h}$, which is determined through yet another minimization problem and influenced by the evolution of the enthalpy that is not known prior to the start of the evolution

[13] More information on this benchmark can be found here:
http://people.aifb.kit.edu/jbr/MovPeaks/movpeaks.

[14] Those are optimization algorithms that work, in each search iteration, with a group of current solution candidates rather than just one (Onwubolu and Babu, 2004). For example, genetic algorithms (Goldberg, 1989) or algorithms based on swarm intelligence as stochastic diffusion search (Bishop, 1989) or particle swarm optimization (Kennedy and Eberhart, 1995) fall into this category.

[15] Following (Benešová, 2008; Kružík et al., 2005; Roubíček et al., 2007), we implemented the *L-BFGS-B* algorithm (Byrd et al., 1995; Zhu et al., 1997), a limited memory gradients descent algorithm allowing for bounds. The gradients for this algorithm are provided by automatic differentiation through the *ADOL-C* routine (Walther et al., 2003), for more information on automatic differentiation see e.g. the works (Griewank et al., 2000; Griewank and Walther, 2008) by the authors of ADOL-C.

[16] Simulated annealing was first proposed in (Černý, 1985; Kirkpatrick et al., 1983) and we implemented a variation of this algorithm that follows the ideas described in the preliminary work, only the neighborhood determination is altered to suit the given problem. Namely, a state from the neighborhood

not population based and the population-based *particle swarm optimization method*[17]. As can be seen from calculations in Subsection 7.2.3 the population-based particle swarm optimization routine outperforms simulated annealing that, again, performs better than the local gradient descent.

Remark 7.9 (Tailoring particle swarm optimization to dynamic environments). Let us note that the population-based particle swarm optimization method has originally been proposed for minimization in non-changing environments, however extensions exist also for dynamic environments (e.g. (Blackwell, 2003)). The authors of these generalizations are generally concerned with the question on how to alter the swarm in every time-step – two extremal approaches lie at hand: erase all information from all particles and practically restart the whole minimization ignoring all information obtained about the shape of the cost function in the last time-step or, on the other hand, keep the *same* swarm (with the same history) relying on the idea that the particles will react to the change of the cost function and find the changed global optimum. While the first approach is not effective, the second might not work.[18] So, in our situation we use some compromise between the two approaches (however nearer to the first extremum, since we are unable to estimate how large the change of the cost function will be in every time-step) through an appropriate choice of the initial guess.

Remark 7.10. Most of the existing, and in particular the three implemented, minimization algorithms are iterative and need an *initial guess*. By an initial guess we mean either a single state in the state space from which the iteration starts (as for e.g. gradient-descent, simulated annealing, tabu search) or an initial distribution of particles (as for e.g. particle swarm, ant-optimization, stochastic diffusion) depending on the selected minimization method . By choosing the initial guess *according to* another state in the state space S (typically a optimum in some time-step) we mean that this initial guess is equal to S if the minimization method requires a single state as initial guess. If the method requires an initial distribution of agents, then we choose the positions of all but one agent randomly in some neighborhood of S. The initial position of one single agent is then equal to S.

7.2.2 Backtracking and multigrid methods

Recall, that we assume that the spatial-discretization is the same throughout the evolution. Then, from (7.7) *if* $\alpha = 0$, i.e. *if we are treating the rate-independent case*, we can deduce the following inequalities by the same procedure as when deducing 4.35 in

of a given state is chosen by changing one random component of the state vector.

[17] The particle swarm optimization method is a *heuristic*, *stochastic*, *derivative-free global optimization* method. It works iteratively, when in each step it modifies the *positions* and *velocities* of current candidate solutions, referred to as *particles*, based on their own current position and the positions of (some) other particles from the swarm. The method has been proposed in (Kennedy and Eberhart, 1995) and has been widely applied since then (see e.g. the monograph (Clerc, 2006)). For our purposes, we implemented the standard particle swarm optimization (2006) (see `http://www.particleswarm.info/Standard_PSO_2006.`) with the change that each particle has knowledge about the best position found by the whole swarm.

[18] Usually, one encounters the problem of *outdated memory* (i.e. the history particles remember is no longer valid due to the change of the environment) and the problem of *lost diversity* (i.e. due to the fact that the swarm has converged all particles have been drown to a small area) (Blackwell, 2003; Hu and Eberhart, 2002).

the proof Proposition 4.3,

$$\int_{t_{k-1}}^{t_k} \partial_t \mathfrak{G}(t, y^k_{\tau,h}, \nu^k_{\tau,h}, \lambda^k_{\tau,h})\,\mathrm{d}t$$
$$\leq \mathfrak{G}(t_k, y^k_{\tau,h}, \nu^k_{\tau,h}, \lambda^k_{\tau,h}) + R(\lambda^k_{\tau,h} - \lambda^{k-1}_{\tau,h}) - \mathfrak{G}(t_{k-1}, y^{k-1}_{\tau,h}, \nu^{k-1}_{\tau,h}, \lambda^{k-1}_{\tau,h}), \quad (7.10)$$
$$\mathfrak{G}(t_k, y^k_{\tau,h}, \nu^k_{\tau,h}, \lambda^k_{\tau,h}) + R(\lambda^k_{\tau,h} - \lambda^{k-1}_{\tau,h}) - \mathfrak{G}(t_{k-1}, y^{k-1}_{\tau,h}, \nu^{k-1}_{\tau,h}, \lambda^{k-1}_{\tau,h})$$
$$\leq \int_{t_{k-1}}^{t_k} \partial_t \mathfrak{G}(t, y^{k-1}_{\tau,h}, \nu^{k-1}_{\tau,h}, \lambda^{k-1}_{\tau,h})\,\mathrm{d}t, \quad (7.11)$$

where we shall refer to (7.10) as the *lower energy inequality* while we shall call (7.11) the *upper energy inequality*. Let us note that, whereas an equivalent to (7.11) could be deduced also from (7.6b), (cf. 5.112); the inequality (7.10) relies on solving (7.7) in the *rate-independent* case.

Let us, thus, restrict our attention to the rate-independent case in which we are searching for solutions to (7.7) – as (7.10)-(7.11) form some *zero-order* necessary conditions for solutions to (7.7), one can enhance the search for of solutions to (7.7) by verifying the estimates in every time-step; within this section, we propose a *backtracking* strategy based on (7.10) and a *combined backtracking and multigrid* strategy based on (7.11). Furthermore, let us stress that, not only this verification enhances optimization, but it also *assures conservation of energy*, a fundamental physical principle.

Finally, let us just remark that the backtracking strategy *cannot* be applied to the *rate-dependent* (7.6b) (since an equivalent of (7.10) is missing) while the multigrid strategy could be used if, of course, backtracking is omitted on both the fine and the coarse mesh.

The strategy of backtracking has already been used before in the context of rate-independent processes in (Mielke et al., 2010) in a damage problem. The combined strategy of backtracking and multigrid, was first presented in (Benešová, 2011*a*) obtained within the work on this thesis.

Backtracking strategy

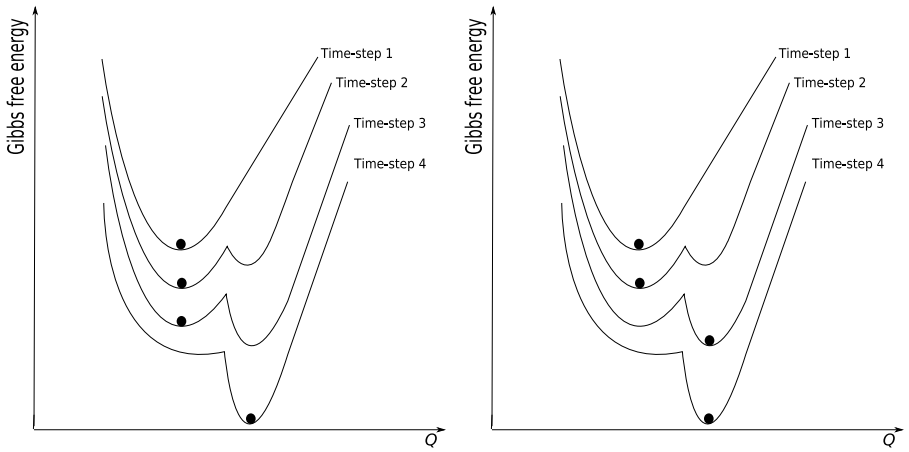
From the proof (7.10) (see (Benešová, 2011*a*; Francfort and Mielke, 2006)), we can deduce that (7.10) verifies whether the optimum found in the k-th step would not give a smaller value of the cost function in the $(k-1)$-th step than the optimum found there; i.e. it verifies whether the minimization algorithms was not trapped in a local minimum in the $(k-1)$-th step which could only be escaped in the k-th step.

For example, suppose that our aim is to minimize the energy[19] that initially was a convex function with one global minimum. In the next time-step a further local minimum emerges, which becomes global in time-step 3 and 4; the situation is schematically depicted in Figure 7.2. In this Figure, the black dot represents the state found as optimal by a local search algorithm [20] with a choice of initial guesses as chosen according to the optimum found in the last step, cf. Remark 7.10. Since the algorithm stays trapped in the local minimum in step 3 and escapes it only in step 4, in step 4 the lower energy inequality would not be satisfied.

Assume that the initial guess for an (iterative) optimization method is chosen according to the optimum from the last step, cf. Remark 7.10. If then the lower energy inequality is not satisfied, the following strategy of "backtracking" will be used: the algorithm returns to the previous time-step and the initial guess is given to the algorithm according to the current state $q^k_{\tau,h}$ – schematically this is shown in Figure 7.3.

[19] Let us omit the dissipation, for simplicity.

[20] Even using a population-based algorithm could lead to the same result, if the region in which the



(a) Situation without backtracking (b) Situation with backtracking

Figure 7.2: Example of an evolution of the energy when the two-sided energy inequality will not be satisfied, the black dot denotes the state evaluated as optimal by the algorithm.

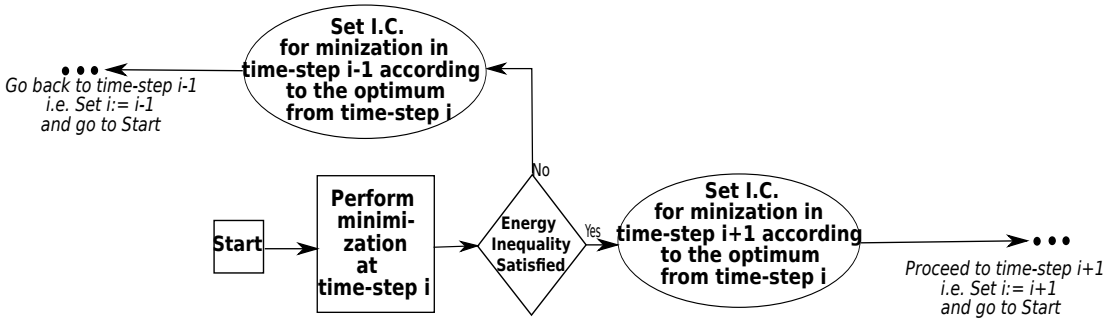


Figure 7.3: A scheme of the strategy of backtracking shown on one specific time-step. The arrows show the proceeding of the algorithm.

Note that if (7.10) was not at our disposal, we could not decide whether it is sensible to perform backtracking in the current step. Of course, one could try to backtrack "preventively" in every time-step, but this would be *very ineffective*. To this end, let us also remark that it *would not* help, if we could establish (an equivalent to) (7.11) since this inequality is satisfied *automatically* if the initial guess is chosen *according* to the last step's optimum.

Finally, let us remind the reader that backtracking strategies are well known when searching for an optimizer of some objective ((Golomb and Baumert, 1965) or e.g. (Bourdin, 2007; Bourdin et al., 2008)) or more generally when solving computational problems in which solutions are build incrementally – it was first introduced in (Walker, 1960). In the general setting, a satisfaction criterion is found the partial solution has to satisfy; the solution vector is then constructed according to this criterion. If there are, however, no admissible solution in the k-th step satisfying the satisfaction criterion, one has to backtrack one or several steps and select some components of the partial solution vector differently to be able to fulfill the satisfaction criterion in the k-th step. In our case this criterion is (7.10) – in contrast to the general case however, our method provides a hint on how to construct the preceding states when backtracking is needed; in the general setting the preceding states are chosen randomly.

initial population is distributed was too small.

Combined backtracking and multigrid strategy

Particularly on fine meshes, where the number of degrees of freedom of the minimization algorithm is huge,[21] a local search algorithm may escape the "local minimum trap" only after a very long time (and perhaps never) – in such a case, (7.10) is satisfied until some local minimum is escaped, so it looses its selectivity.

Moreover, using population-based methods on fine-meshes is *very* time-consuming, since the number of particles has to increase with number of degrees of freedom to allow these methods to effectively search in the state space.

Thus, we propose a straightforward, but effective strategy that can be used to handle fine meshes – namely, the strategy of successive refinement of meshes referred to as *multigrid strategy*, possibly combined with backtracking. This strategy falls into the category of *multilevel methods* that were first introduced in the context partial differential equations (Brandt, 1977), but later also applied to optimization problems (see e.g. (Hager et al., 2006)), here of course we adapted the strategy to our context. Let us remark that the multigrid strategy can be applied *to the rate-independent case* governed through (7.7) (here it can be combined with backtracking) *as well as to the rate-dependent case* governed through (7.6a)-(7.6b) since an equivalent to (7.11) is available in this case.

To be more specific, the multigrid strategy works as follows: first the simulation is run on a coarser mesh; the strategy of backtracking is used throughout the calculation, if appropriate. Then the simulated optimal states are extrapolated to a finer mesh. Of course, the extrapolation has to suit the numerical discretization, here we, e.g., extrapolate piecewise affine variable by affine interpolation whereas piecewise constant variables are interpolated constantly. The initial guess while running the simulation on the finer mesh is then given to the algorithm according to this extrapolated state in each time-step.

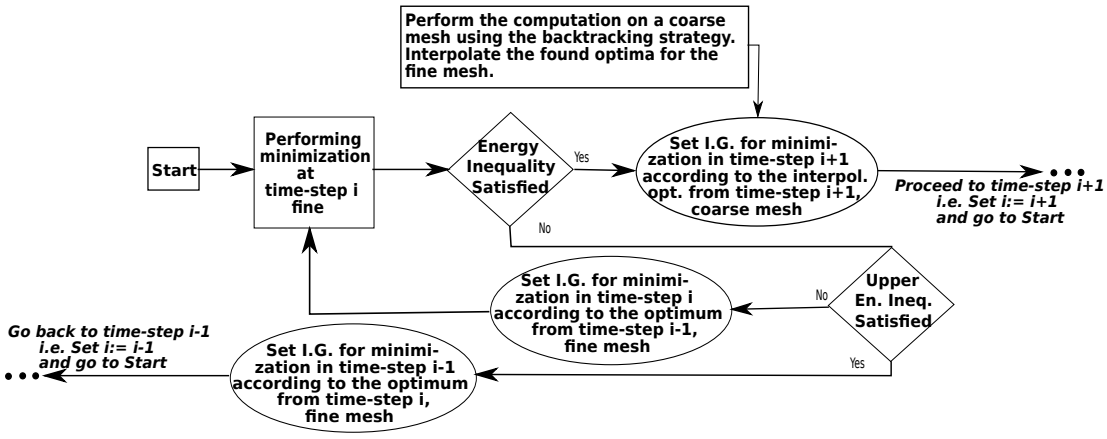


Figure 7.4: A scheme of the multigrid strategy combined with backtracking shown on one specific time-step. The arrows show the proceeding of the algorithm.

Again, during the second simulation on a finer mesh, the strategy of backtracking is still used[22], however needs a little bit more care because we need to distinguish between the violation of (7.10) and (7.11). In the former case, we proceed standardly as before; in the latter case however the current time-step is minimized once again, but now using an initial guess according to the optimum found in the last step on the

[21] On the meshes we call *fine* in this section, the dimension of the state space reaches the order of thousands, which, for global optimization, is an extremely large state space.

[22] Clearly, only in the *rate-independent setting* when (7.10) is at our disposal

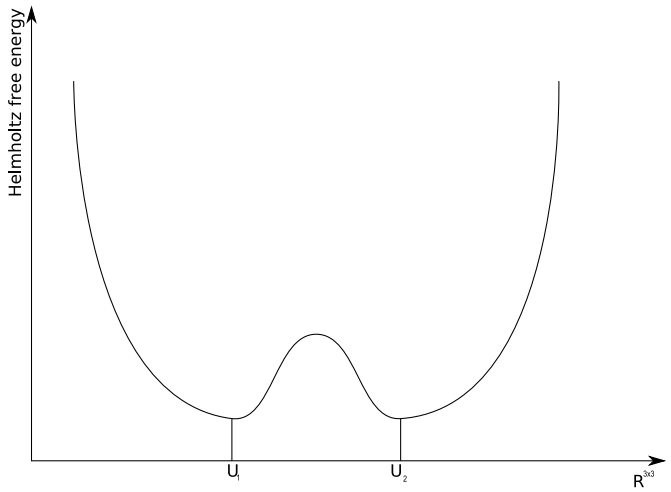


Figure 7.5: A typical landscape of a 2-well potential. Here for simplicity the space $\mathbb{R}^{3\times 3}$ is shown only one-dimensional

fine discretization – the situation is schematically shown in Figure 7.4. Finally, let us remark that violation of (7.11) is handled the same way, even if backtracking is not available.

7.2.3 Computational examples

As already announced in the introduction to this chapter, we test the proposed algorithms on the so-called two-well problem – this corresponds to choosing $m = 2$ in Remark 7.5; for illustration, ϕ_1 corresponding to this choice is depicted in Figure 7.5. Following (4.6) and Figure 7.5, we denote the matrices at which the wells of ϕ_1 lie as U_1, U_2 and assume moreover that U_1 and U_2 are rank-1 connected, i.e. satisfy 2.27. Note that the two-well potential is perhaps the simplest representant of a non-convex Helmholtz free energies used in mesoscopic SMA modelling that still brings most of the relevant difficulties with it – physically U_1 and U_2 correspond to two variants of martensite. Also, let us remind the reader that the calculations here we performed within the *rate-independent setting* using (7.7).

The computations are then performed within the code described in Section 7.1, when choosing the order of lamination ℓ as 1. Finally, we add that the graphs representing the results have been reprinted from (Benešová, 2011*a*).

Simulations on a coarse 18-element mesh

To examine the efficiency of the algorithm depicted in Figure 7.3 (and the efficiency of stochastic and/or population based minimization), we perform the following loading experiment: we take a, initially stress free, cuboid specimen subject to a volume force increasing in time, at two opposite faces, however, zero Dirichlet boundary conditions for the displacement are prescribed. Further, we divide the evolution into 2000 time-steps and introduce a 18-elements mesh[23]; in each time-step we prescribe the initial guess for the used iterative minimization algorithms according to the optimum found in the last step.

As for minimization algorithms, we compare all three implemented algorithms i.e. gradient-descent, simulated annealing and particle swarm optimization – we expect that

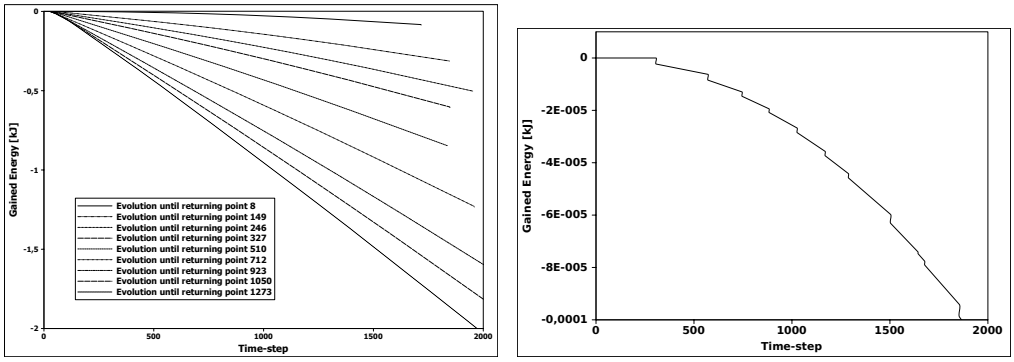
[23] This leads to approx. 150 degrees of freedom for minimization.

the latter two will need less backtracking work, since they have the ability to escape local minima.

To illustrate the effectiveness of backtracking when using gradient-descent, we give, in Figure 7.6, a comparison of the *gained energy* evolution[24] in the case when backtracking is used as well as in the case when it is not. Clearly, the energy is (more than 1000 times) lower when using the strategy of backtracking compared to the case when it is not.

Notice that the points where backtracking starts are characterized within the gained energy evolution (compare Figure 7.6 on the right) by "deep falls" of the gained energy – these deep falls correspond to escaping of the local minimum trap.

Finally, we add that, due to the large amount of backtracking work, the calculation of the whole evolution took approximately one week on a ordinary PC.



(a) backtracking (b) no backtracking

Figure 7.6: Comparison of the gained energy evolution on a coarse 18-element mesh using gradient-descent as minimization algorithm. On the right the strategy of backtracking has not been used, on the left it has. In the case when backtracking is used, we use the name *returning point* for a point in the calculation in which backtracking has been yielded; thus, the e.g. the returning point 327 corresponds to the point when backtracking is used for the 327-th time in the calculation. Note that the scaling of the y-axis on the left and on the right is different.

Remark 7.11 (Comparison to (Mielke et al., 2010)). As already seen from Figure 7.6, the number of *returns* (i.e. the number of times when backtracking is started) in the presented simulation is huge and reaches more than 1000. This number is especially striking when compared to the first usage of an algorithm similar to the one depicted in Figure 7.3 in (Mielke et al., 2010)[25], where only one return has been observed. Also, in (Mielke et al., 2010) the strategy of backtracking has been useful to calculate the intermediate states between the start of the calculation and the returning point. In time-steps following this point the calculated states would not be affected by verification of the two-sided energy inequality and backtracking. Yet, in the case of the two-well problem, the situation is completely different. *Only* due to backtracking the algorithm "gets on the right track" – the results are completely different in all time-steps when the strategy of back-tracking is used compared to when it is not.

When using *simulated annealing* as minimization procedure, again a huge amount of backtracking, namely 660 returns, were needed. Still, in comparison with the case when using gradient descent for minimization, this amount could be reduced to a half.

[24] By the *gained energy* we understand the cost function in (7.7) for some time-step k.

[25] In (Mielke et al., 2010) also a gradient descent algorithm was used; however, since the cost function was separately convex an altering directions algorithm due to (Bourdin, 2007; Bourdin et al., 2008) could be exploited.

Yet, because one iteration using simulated annealing took longer, it took two weeks on a usual PC to perform the computation.

Rather then comparing the gained energy evolution in the case when simulated annealing is used as minimization algorithm (with and without backtracking), we shall give a comparison of the microstructure[26], which we present in Figure 7.9. In this figure a comparison of the evolution of the volume fraction is shown by the gray-scale of the specimen; the wireframe on this specimen indicates the used mesh. The microstructure on two selected elements is shown on two separate cubes; the chosen elements are indicated by arrows.

Within the simulation using *particle swarm optimization*, backtracking work could be significantly lowered, in fact only 50 returns were observed.[27] This is demonstrated also in Figure 7.7 where an evolution of the overall gained energy is presented – we see that the gained energy value after 80 time-steps when using and when not using backtracking are much nearer to each other than when using gradient descent. On the other hand, since one iteration took longer than in the preceding two cases, it took 4-5 days to perform the calculation on an ordinary PC.

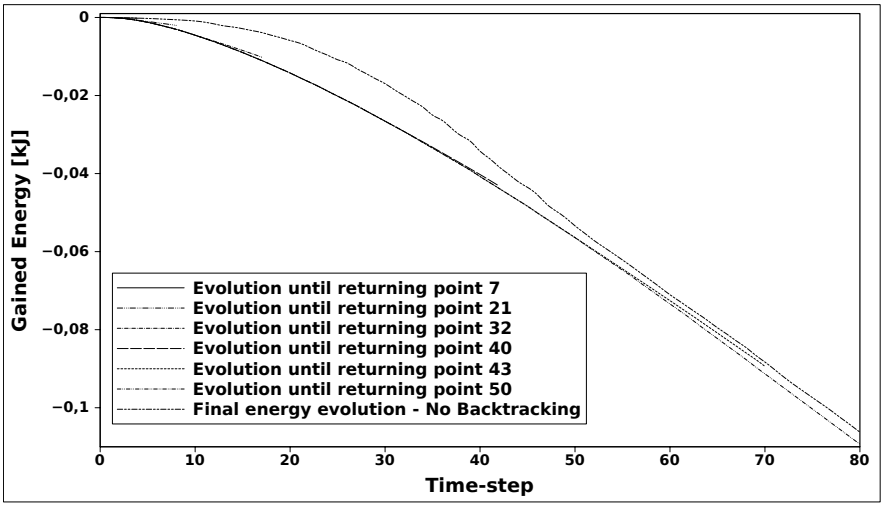


Figure 7.7: Energy evolution using particle swarm optimization. The energy when using and when not using backtracking is given.

To decide which algorithm is best suited for our purposes, we compare the *final*[28] gained energies in Figure 7.8; it can be clearly seen that while particle swarm optimization and simulated annealing lead to practically identical results, they both outperform the gradient-descent which is, again, connected to their ability to escape from local minima traps.[29]

When turning to computation time, particle swarm optimization as minimization routine yielded the fastest computation, the second fastest was the usage of gradient-descent and the slowest the usage of simulated annealing. However, as the number of swarming particles is dependent on the dimension of the state space, for finer meshes

[26]The evolution of the gained energy is (qualitatively) very similar to the one given for the case when using gradient descent, and, on the other hand, the evolution of the microstructure when using simulated annealing is similar to the one when using gradient descent. So, we give each evolution calculated by a different minimization algorithm.

[27]A reason for not needing so much backtracking work, is our choice to take the initial position of all but one particles randomly in every time-step. It is probable that if we chose randomly a smaller part of the population as in (Hu and Eberhart, 2002), more backtracking work would be required.

[28]I.e. after all backtracking is completed.

[29]For the same reason, the amount of backtracking work is lowered.

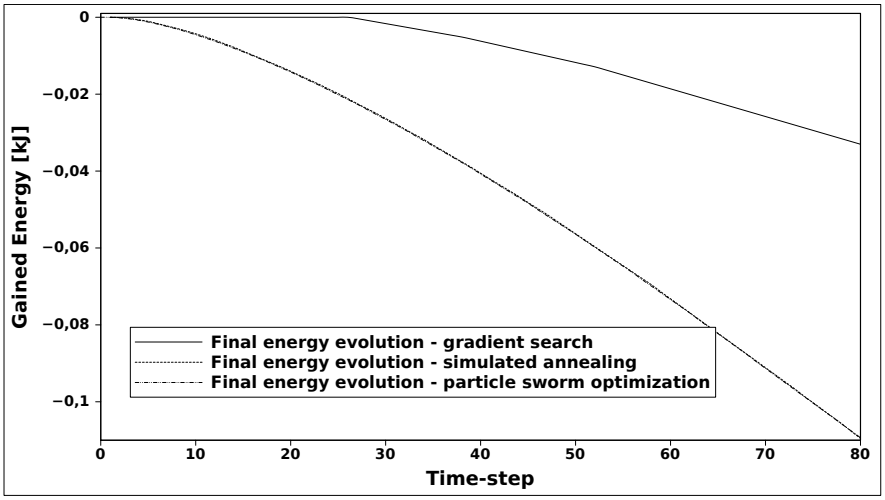


Figure 7.8: Comparison of the evolution of the gained energy when using three different minimization routines.

the calculation using this minimization routine could be very slow – this could be resolved by implementing a multigrid as in Figure 7.4 using an agent-based method on the coarse mesh and simulated annealing or gradient-descent on the fine mesh.

Simulations on a fine 144-element mesh

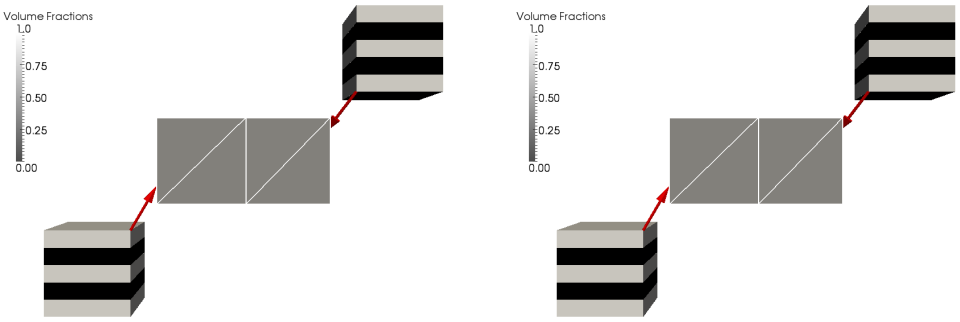
On the fine 144-element mesh[30] we exploit the strategy from to Figure 7.4; i.e., we use the results of the simulation using particle swarm optimization from the calculations on the 18-element mesh, extrapolated adequately, as initial guesses in a calculation using the same data as in the previous section but performed on a finer 144-element mesh. For the sake of verification, we performed the same calculation also in a standard manner following the algorithm depicted in Figure 7.3 and not using calculations on the coarser mesh at all. In both cases we used gradient-descent as minimization routine.

A first difference between the two approaches is in computation time: whereas the simulation using the multigrid strategy took about one day and brought satisfactory results[31] the strategy following just the algorithm depicted in Figure 7.3 was interrupted after three weeks, still not giving satisfactory results.

Also, Figure 7.10, showing the comparison of the microstructure evolution when the multigrid strategy has and has not been used, shows the effectiveness of the multigrid method. Indeed, when not using the multigrid strategy, the phase transition starts at a later point and does not complete in the two thirds of the specimen until the end of the loading cycle; in the case when we employed the multigrid strategy the phase transition *did* complete.

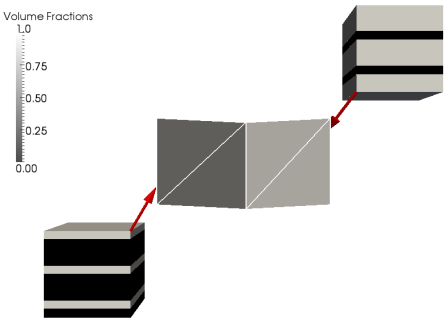
[30] The mesh is called fine, since the number of degrees of freedom is 1260, which is a large number for minimization.

[31] Here the time needed for the calculation on the coarse mesh is not included; if counted, the computation time is about one week.

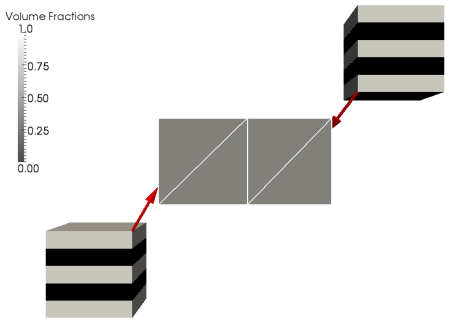


(a) Time-step 0, back-tracking

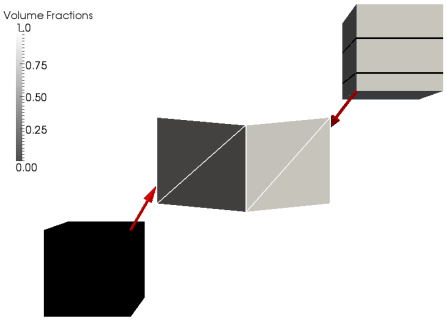
(b) Time-step 0, no back-tracking



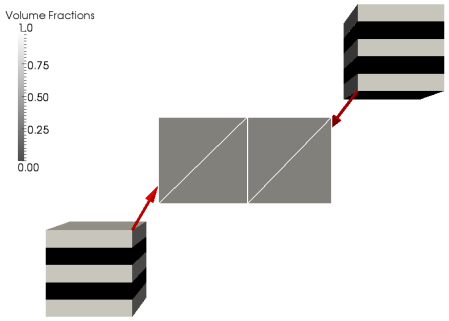
(c) Time-step 15, back-tracking



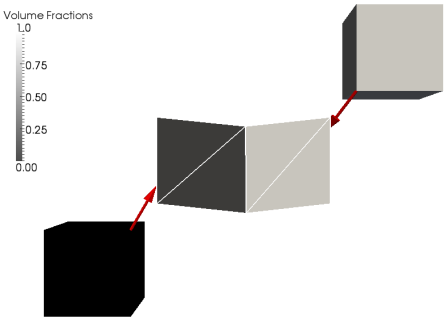
(d) Time-step 15, no back-tracking



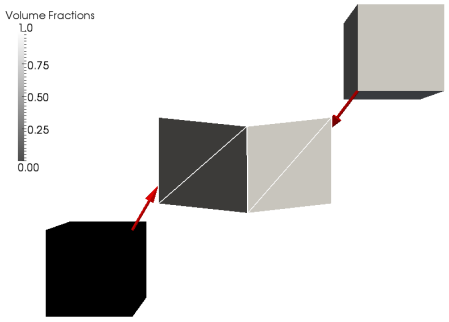
(e) Time-step 99, back-tracking



(f) Time-step 99, no back-tracking



(g) Time-step 660, back-tracking



(h) Time-step 660, no back-tracking

Figure 7.9: Comparison of the evolution of volume fractions and microstructure on a coarse 18-element mesh using simulated annealing as minimization routine. On the right the strategy of backtracking has not been used, on the left it has.

7.3 Illustration: Computation in thermally case for the two-well problem

To illustrate, at least qualitatively, the capabilities of the mesoscopic thermally coupled model for SMAs devised within this thesis in Chapter 5 as well as its computer implementation, we provide in this section computed results for the two-well problem as already introduced in the beginning of Subsection 7.2.3.

Furthermore, we make the assumption that the phase corresponding to well the U_1 is preferred at higher temperatures, while the phase U_2 is preferred at lower ones. In particular, we assume that the phase corresponding to U_2 is stable below 10K, while U_1 is stable above this temperature – i.e., in this setup, $\theta_{\text{tr}} = 10$.[32] We chose this setup since it represents the *simplest possible way* to simulate the *mechanical deformation due to phase transition* that was induced by heat supply.

Let us stress, however, that our setup *does not* correspond to a crystalline structure of any SMA-material because in none of the known SMA materials the matrix representing the austenite phase can be rank-1 connected to the matrix representing some variant of martensite. Nevertheless, including more wells, which would correspond to physically relevant cases, bears even more non-convexity than the two-well problem and requires time-consuming computations and possibly even more optimization than was done so far. Yet, principally, the developed code presents a good basis to launch even these lengthy computations. As, in this thesis, emphasis was laid mainly upon the mathematical analysis of thermally coupled model for SMAs (5.17), we believe that presenting calculations only for the illustrative two-well problem is sufficient.

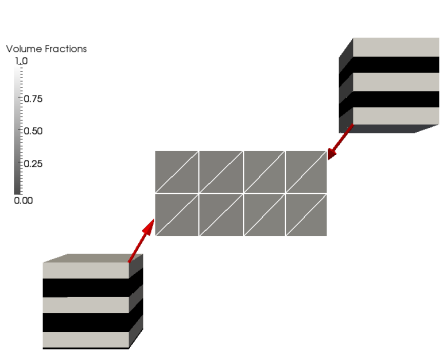
During all simulations we solve (7.6a)-(7.6c) with the order of lamination chosen as 1. To improve the search for global optima of (7.6b) we exploit a *particle swarm optimization algorithm*; however, as outlined in Section 7.2, the strategy of backtracking is not available for this situation. As far as meshing is concerned, we use a coarse mesh having 18 elements.

We chose, for illustration, a canonical loading experiment in which thermo-mechanical coupling manifests itself. Initially, the specimen is held at transformation temperature θ_{tr} and consists of a laminate of the phases described by the matrices U_1 and U_2. In 150 sequential time-steps then a (negative) heat flux is applied on the upper face of the boundary that gradually cools the specimen from 10K to 9.8K, which forces it to transform to the phase U_2.

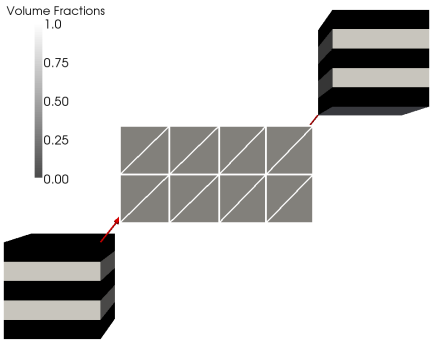
The results of the simulation are shown in Figure 7.11; there the same specimen is shown, with a wireframe representing meshing, two times next to each other – on the right the specimen is coloured according to the temperature in the specimen, on the left according to the volume fraction of U_1. On the left in the bottom the microstructure on one chosen element is shown – the selected element is indicated by an arrow.

It can be observed that the negative heat flux cools the upper elements first, so they transit first into the phase U_2 and force a deformation in the upper elements. Ones the negative heat spreads to the lower elements, these transform as well.

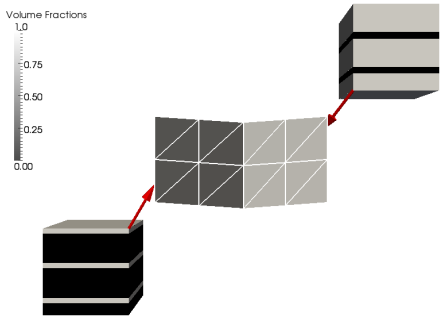
[32] Of course, the transformation temperatures of common SMAs *do not* lie so low. However, as explained below, the two well setup does not correspond to physical SMAs, so we are entitled to choose any arbitrary value here.



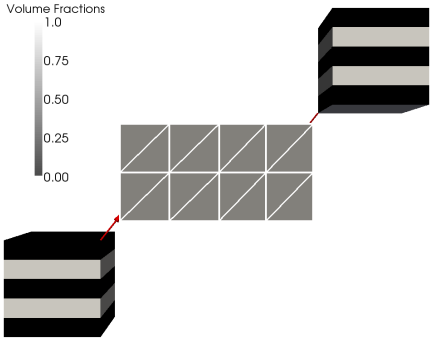
(a) Time-step 0, multigrid



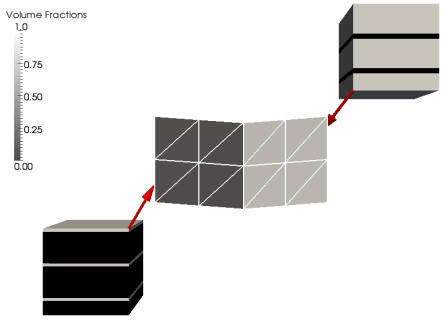
(b) Time-step 0, no multigrid



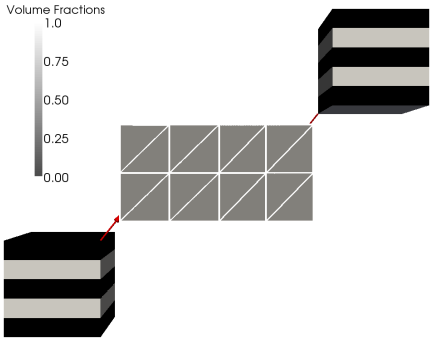
(c) Time-step 30, multigrid



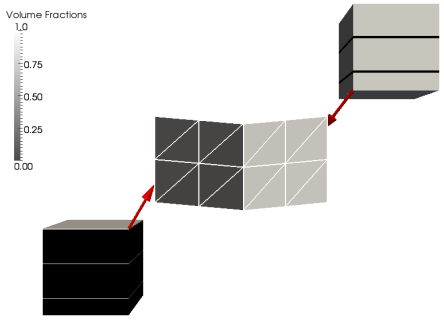
(d) Time-step 40, no multigrid



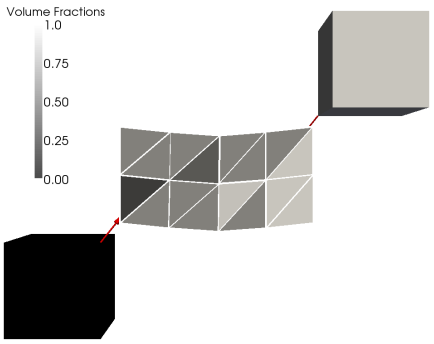
(e) Time-step 40, multigrid



(f) Time-step 230, no multigrid

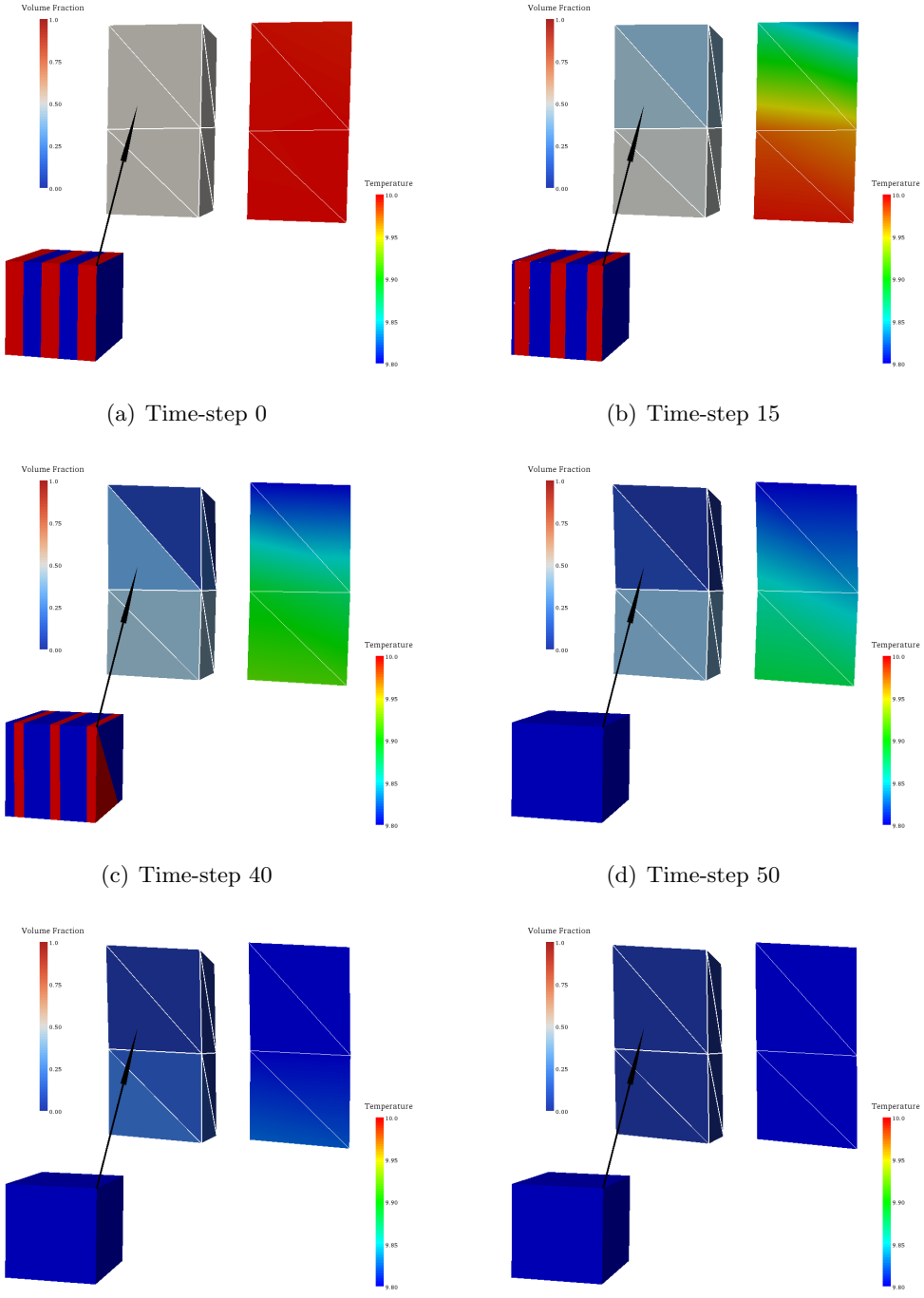


(g) Time-step 130, multigrid



(h) Time-step 1200, no multigrid

Figure 7.10: Comparison of the evolution of volume fractions and microstructure on a fine 144-element mesh. On the right the multigrid strategy has not been used, on the left it has. Note that the time-steps depicted on left and right are different.



(a) Time-step 0

(b) Time-step 15

(c) Time-step 40

(d) Time-step 50

(e) Time-step 70

(f) Time-step 150

Figure 7.11: Phase transition induced by cooling. Here a negative flux is applied on the upper face of the specimen that gradually forces a phase transition.

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