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Mathematical modelling of thin films of martensitic materials

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Supervisor:	Doc. RNDr. Martin Kružík, Ph.D.
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DISERTAČNÍ PRÁCE

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Matematické modelování tenkých filmů z martenzitických materiálů

Matematický ústav

Vedoucí práce:	Doc. RNDr. Martin Kružík, Ph.D.
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Prague, 7th August 2015 Gabriel Pathó

Název práce: Matematické modelování tenkých filmů z martenzitických materiálů

Autor: Gabriel Pathó

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Abstrakt: Cílem této práce je matematické a počítačové modelování tenkých filmů martenzitických materiálů. Dvoustupňovém postupem odvodíme mezoskopický termodynamický model pro tenké filmy, jenž umí zachytit evoluční proces efektu tvarové paměti. Nejprve provedeme redukci dimenze v mikroskopickém 3D modelu, pak zvětšíme měřítko zanedbáním mikroskopických mezifázových vlivů. Počítačové modelování tenkých filmů je provedeno v statickém případě zahrnutím modifikované Hadamardovy podmínky skoku, jež dává slabší podmínku na kompatibilitu fází ve srovnání s 3D modelem. Dále jsou popsány L^p-Youngovy míry generované regulárními maticemi, popř. maticemi s kladným determinantem. Gradientní případ je vyřešen pro zobrazení, kde gradient a inverze gradientu jsou v L^∞, netriviálním problémem byla manipulace s okrajovými podmínkami u generující posloupnosti, neboť standardní "ořezávací metody" nelze v našem případě aplikovat kvůli podmínce na determinant. V poslední kapitole zmíníme nové výsledky týkající se slabé zdola polospojitosti integrálních funkcionálů podél tzv. (asymptoticky) $\mathcal{A}$-free posloupností, jež mohou být záporné i nekoercivní.

Klíčová slova: materiály s tvarovou pamětí; redukce dimenze; rychlostně nezávislá evoluce; Youngovy míry; slabá zdola polospojitost

Title: Mathematical modelling of thin films of martensitic materials

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Abstract: The aim of the thesis is the mathematical and computer modelling of thin films of martensitic materials. We derive a thermodynamic thin-film model on the meso-scale that is capable of capturing the evolutionary process of the shape-memory effect through a two-step procedure. First, we apply dimension reduction techniques in a microscopic bulk model, then enlarge gauge by neglecting microscopic interfacial effects. Computer modelling of thin films is conducted for the static case that accounts for a modified Hadamard jump condition which allows for austenite–martensite interfaces that do not exist in the bulk. Further, we characterize L^p-Young measures generated by invertible matrices, that have possibly positive determinant as well. The gradient case is covered for mappings the gradients and inverted gradients of which belong to L^∞, a non-trivial problem is the manipulation with boundary conditions on generating sequences, as standard cut-off methods are inapplicable due to the determinant constraint. Lastly, we present new results concerning weak lower semicontinuity of integral functionals along (asymptotically) $\mathcal{A}$-free sequences that are possibly negative and non-coercive.

Keywords: shape-memory alloys; dimension reduction; rate-independent evolution; Young measures; weak lower semicontinuity

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Notation

M	number of different martensite variants
θ_{tr}	transformation temperature below which the martensite is stable, above which the austenite
U_i	transformation matrix of the austenite for $i = 0$, of the different martensitic variants for $i = 1, \dots, M$
$\mathcal{I}$	the identity matrix in $\mathbb{R}^{n \times n}$
$F^\top$	the transpose matrix of $F \in \mathbb{R}^{n \times n}$
$\mathcal{L}$	phase indicator function $\mathbb{R}^{3\times 3} \to \mathbb{R}^{M+1}$ such that $[\mathcal{L}(F)]_i = 1$ when F is in the (vicinity of) the i-th variant / phase, it holds that $\sum_{i=0}^{M} \mathcal{L}_i = 1$
δ_K^*	the Legendre–Fenchel conjugate of the indicator function of a convex set K
$O(d)$	orthogonal group $O(d) = \{Q \in \mathbb{R}^{d\times d} \colon Q^\top Q = QQ^\top = I\}$
$SO(d)$	special orthogonal group $SO(d) = O(d) \cap \{Q \in \mathbb{R}^{d\times d} \colon \det Q = 1\}$
Ω	the reference domain, an open bounded domain in $\mathbb{R}^3$ with Lipschitz boundary
Γ_D	open subset of $\partial\Omega$ where Dirichlet boundary condition is prescribed
Γ_N	boundary part with prescribed Newton boundary condition, there is $\partial\Omega = \Gamma_D \cup \Gamma_N$ up to a null set
$\Omega_\varepsilon, \omega$	$\Omega_\varepsilon = \omega \times (-\varepsilon/2, \varepsilon/2)$, where $\omega \subset \mathbb{R}^2$ an open bounded domain with Lipschitz boundary, the plane of the film, see Chapters 2 and 3
z_p	the in-plane component (z_1, z_2) of a point $z = (z_1, z_2, z_3) \in \mathbb{R}^3$
γ_D	boundary part of $\partial\omega$ such that $\Gamma_D = \gamma_D \times (-\varepsilon/2, \varepsilon/2)$
γ_N	boundary part of $\partial\omega$ such that $\Gamma_\varepsilon = \gamma_N \times (-\varepsilon/2, \varepsilon/2)$
$[0, T]$	finite time interval of the evolutionary problems
Σ^ε	$= [0, T] \times \partial\Omega_\varepsilon$
Σ_D^ε	$= [0, T] \times \Gamma_D^\varepsilon$, where $\Gamma_D^\varepsilon \subset \Omega_\varepsilon$, see the definition of Γ_D
Σ_N^ε	$= [0, T] \times \Gamma_N^\varepsilon$, where $\Gamma_N^\varepsilon \subset \Omega_\varepsilon$, see the definition of Γ_N

$C(M;\mathbb{R}^m)$	set of continuous functions $f\colon M \to \mathbb{R}^m$ (here and in the following function spaces for $m=1$ we suppress $\mathbb{R}$ and write only $C(M)$)
$C^k(M;\mathbb{R}^m)$	set of k times continuously differentiable functions, $k \geq 1$; C^∞ denotes the set of continuously differentiable functions up to any order
$C_0(\mathbb{R}^{m\times n})$	set of $f \in C(\mathbb{R}^{m\times n})$ vanishing at infinity
$C_p(\mathbb{R}^{m\times n})$	set of $f \in C(\mathbb{R}^{m\times n})$ such that $f(s) = o(\lvert s\rvert^p)$ for $\lvert s\rvert \to \infty$
$\mathrm{rca}(\mathbb{R}^{m\times n})$	space of regular countably additive measures on $\mathbb{R}^{m\times n}$, it is isometrically isomorphic with the dual space $(C_0(\mathbb{R}^{m\times n}))^*$
$L^p(\Omega;\mathbb{R}^m)$	Lebesgue space of measurable functions $f\colon \Omega \to \mathbb{R}^m$ such that $\lvert f\rvert^p$ is Lebesgue integrable as well
$W^{k,p}(\Omega;\mathbb{R}^m)$	Sobolev space of measurable functions that admit a p-integrable distributional derivative up to order k
p'	the conjugate exponent $p' := \begin{cases} p/(p-1) & \text{for } 1 < p < \infty, \\ 1 & \text{for } p = \infty, \\ \infty & \text{for } p = 1 \end{cases}$
p^*	having $W^{k,p}(\Omega;\mathbb{R}^m)$ such that $\Omega \subset \mathbb{R}^n$, then the Sobolev exponent $p^* := \begin{cases} np/(n-kp) & \text{for } kp < n, \\ \text{arbitrarily large real} & \text{for } kp = n, \\ \infty & \text{for } kp > n \end{cases}$
$p^\#$	having $W^{1,p}(\Omega;\mathbb{R}^m)$ such that $\Omega \subset \mathbb{R}^n$, then the trace exponent $p^\# := \begin{cases} (np-p)/(n-p) & \text{for } p < n, \\ \text{arbitrarily large real} & \text{for } p = n, \\ \infty & \text{for } p > n \end{cases}$
$W^{-1,p}(\Omega;\mathbb{R}^m)$	the dual space of $W_0^{1,p'}(\Omega;\mathbb{R}^m)$
$L^p(0,T;V)$	Bochner space of Bochner integrable functions $f\colon [0,T] \to V$, V a Banach space, such that $\int_0^T \lVert f(t)\rVert_V^p \,\mathrm{d}t < \infty$; we do not distinguish between $[f(t)](x) \equiv f(t,x)$ if $V = L^q(\Omega;\mathbb{R}^m)$
$W^{1,p}(0,T;V)$	Sobolev–Bochner space $\{f \in L^p(0,T;V)\colon \dot f \in L^p(0,T;V)\}$, with the norm $\lVert f\rVert_{W^{1,p}(0,T;V)} = \lVert f\rVert_{L^p(0,T;V)} + \lVert \dot f\rVert_{L^p(0,T;V)}$ it is a Banach space; , $\dot f \equiv \mathrm{d}f/\mathrm{d}t \equiv \partial f/\partial t$ denotes always the distributional time derivative of f
$BV(0,T;V)$	space of functions with bounded time variation with values in a Banach space V
$B(0,T;V)$	space of functions bounded in time with values in a Banach space V
$\mathcal{Y}^p(\Omega;\mathbb{R}^{m\times n})$	the set of Young measures, see Definition 1.5.1
$\mathcal{G}^p(\Omega;\mathbb{R}^{n\times d})$	the set of gradient Young measures, see Definition 1.5.2

Preface

In first place, the current work is dedicated to the mathematical and computational modelling aspects of martensitic thin films, more precisely of single-crystal specimen on the micro- and mesoscopic scale (Chapters 2 and 3). But not only: beyond this main aim, the author had the opportunity to contribute to closely related topics within the scope of calculus of variations, namely the characterization of (gradient) Young measures generated by invertible matrices (Chapter 4) and weak lower semicontinuity of integral functionals through the so-called $\mathcal{A}$-quasiconvexity at the boundary (Chapter 5).

Depending on their utilization, shape-memory alloys (SMAs) can be modelled on different scales including different levels of complexity. Chapter 1 aims at making clear these approaches both in the bulk and thin films. First, it introduces the principal physical properties of shape-memory alloys that we are mainly interested in, such as the shape-memory effect, quasiplasticity, superelasticity, and shortly discusses the deviations of the micro-, meso-, and macroscopic views on the problem. The mathematical description is then built up beginning at the definition of a Bravais lattice associating to it important features, such as symmetries, austenite and martensite wells, and the corresponding free energy. Through the Cauchy–Born hypothesis we ascend to a continuum mechanical framework that will be the basis of all that follows. Afterwards we review the existing mathematical models for single crystals – more or less in chronological order and increasing complexity requiring more involved tools, such as (gradient) Young measures and the concept of energetic solutions – that form the foundations of our newly derived models.

Chapter 2 displays our new results [15] concerning the establishment and analysis of a martensitic thin film model with thermo-mechanical coupling. To the best of our knowledge this is the first effectively ansatz-free derivation of such an evolutionary (quasistatic) problem. We start from a slight modification of a well-established microscopic bulk model [18] and arrive to the final description after a two-step procedure, when we first reduce the dimension of the problem by limiting the material thickness to zero and then reduce the interfacial-energy contributions to zero as well.

Existence results for martensitic-alloy theories usually involve either the quasiconvex envelope of the energy density or Young measures. Both of these objects lack, however, an effective characterization so that a numerical scheme would be right at hand. The quasiconvex envelope of a function can be approximated from below by the so-called polyconvex envelope and from above by the rank-one convex envelope. In turn, there exists an approximation of this rank-one convex envelope by the so-called sequential laminates, see [48] that is then in most cases used for numerical computations, see [56, 52], among others. These sequential laminates have been exploited also for computational experiments of quasistatic rate-independent evolution of bulk martensitic specimen, see [13, 24, 53]. Thin films, moreover, differ from the bulk. In our interpretation thin films are not merely a slice of a 3D specimen in a given plane, but entail fundamental differences. In a specimen where the austenite phase and/or different variants of the martensite could co-exist next to each other, the so-called Hadamard jump condition has to be fulfilled by an admissible deformation in order not to tear the specimen apart. In three dimensions this imposes a planar constraint, while in thin films a less restrictive constraint along a line – resulting in interfaces that are not compatible in the bulk(for example, any austenite–martensite interface), see [23]. Chapter 3 includes our numerical experiments [66] that reflect on this relaxed constraint, see [22, 54] as well.

In the introduction, we present different techniques to ensure existence of minimizers to the non-(quasi)convex problem of shape-memory-alloy behaviour. Take account of the fact however that each method relies on a p-growth assumption of the free energy, which in turn excludes another natural physical property that any sequence of deformations $\{y_n\}$ such that $\det \nabla y_n \to 0$ should result in a blow-up of the material energy. In his pioneering work Ball [5] showed that polyconvex materials can incorporate this assumption. On the other hand, shape-memory alloys do not fall into this category as their stored energies are not even quasiconvex. Chapter 4 presents our work [16] that treats the aforementioned blow-up condition by considering energies that depend on both the deformation gradient and its inverse. We characterize Young measures generated by sequences of matrices with positive determinant that are together with their inverses bounded in L^p, $1 \leq p < \infty$. The gradient case is much more involved, as the technique of Kinderlehrer and Pedregal [47] heavily relies on cut-off gradients, the invertibility of which cannot be automatically guaranteed. Our results include the L^∞-gradient case, where a workaround has been found through a convex integration method due to Dacorogna and Marcellini [26]. We refer to the recent work [14] that treats additional orientation preservation of bi-Lipschitz planar maps and characterizes the gradient Young measures they generate.

Lastly, in Chapter 5 we present our new results [49] on weak lower semicontinuity of integral functionals where the integrand u satisfies a first-order constant-rank differential constraint $\mathcal{A}u = 0$, this can be viewed as a generalization of the gradient case (take $\mathcal{A} = \text{curl}$) The first results are due to Fonseca and Müller [41], where they analysed non-negative normal integrands and found that $\mathcal{A}$-quasiconvexity is the necessary and sufficient condition granting weak lower semicontinuity of the functional. However, if the integrand is allowed to be negative and non-coercive its behaviour at the domain boundary starts to play an important role as well, see [57, 51] for the gradient case. If the integrand possesses a recession function, then the correct condition is the so-called quasiconvexity at the boundary [8]. We extracted necessary and sufficient conditions for the case of a general first-order constant-rank operator $\mathcal{A}$ both for $\mathcal{A}$-free and asymptotically $\mathcal{A}$-free sequences, for which $\|\mathcal{A}u_k\|_{W^{-1,p}} \to 0$, and discussed their relationship.

Chapter 1

Introduction

Shape-memory alloys (SMAs) have been extensively studied for more then half a century, since 1951 when the martensitic phase transition was first explained in an Au-Cd alloy, as they exhibit significant phenomena both for theoretical and practical purposes, that stems from their intermetallic behaviour. This means that their structure and characteristic properties are not a mere interpolation between the features of their individual components, but are intrinsically different.

The current work focuses on the mathematical and computational modelling aspects of continuum theories of SMA single crystals on the mesoscopic scale through transition from microscopically inspired models and dimension reduction.

In order to achieve this, we give here in Chapter 1 a short sketch of the main physical properties of these alloys that we are interested in, then introduce also the different mathematical theories concerning both bulk SMAs and thin films that led us in the end in some way to the derivation of a thermo-mechanically coupled model for martensitic thin films, see Chapter 2.

1.1 Martensitic phase transformation and its consequences

SMA materials, such as Ni-Ti, Cu-Al-Ni, Cu-Zn-Al or Ni-Mn-Ga alloys, depending on temperature, may exist in two stress-free phases (the high-temperature, high-symmetry phase called austenite and the low-temperature, low-symmetry one called martensite, respectively) and when exposed to certain conditions they undergo a so-called martensitic phase transformation resulting in a non-diffusive change in their crystallographic structure. This is due to the fact that the relative displacement of the atoms is usually smaller than the interatomic distances.

Remarkable features of these alloys include the so-called shape-memory effect, pseudoelasticity, and quasiplasticity, cf. Figures 1.1.1, 1.1.2.

The shape-memory effect (marked by the blue line in Figure 1.1.1) takes place when the austenitic material is cooled down from high temperature through the transformation temperature θ_{tr}, where in a process called self-accommodation the phase transformation occurs and the material is transformed into the twinned martensite (that has many variants due to a lower crystallographic symmetry). When deformed, detwinning takes place that results in one variant of the martensite in the material. By heating the original highly symmetric shape of the

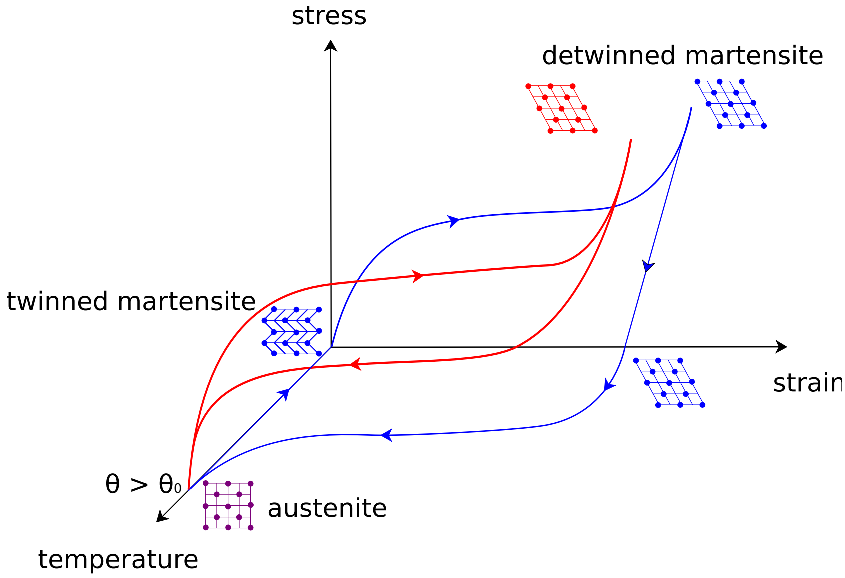

Figure 1.1.1: Shape-memory effect and pseudoelasticity in SMAs

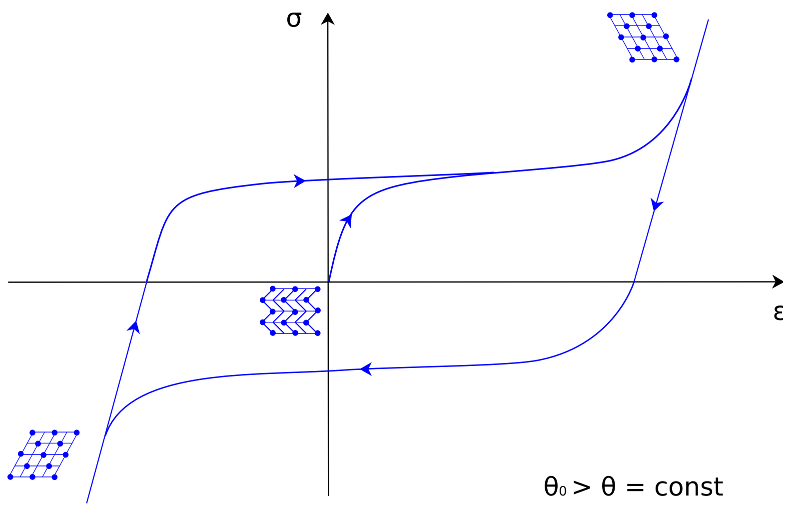

Figure 1.1.2: SMA exhibiting quasiplasticity

austenite is recovered through the reverse transformation.

We can observe the pseudoelasticity of SMAs (red line in Figure 1.1.1) under external load of the austenitic material: around hundreds of MPas – the corresponding stress depends also on the temperature – during phase transformation an extensive elongation of the material (~ 6–7%) occurs for little relative change in the stress (in classic metallic alloys this value is around 0.7%), that explains why sometimes instead of pseudo- the prefix super- is used. The process ends with the material in the detwinned martensite, meanwhile unloading the stress returns the material into the initial austenite.

Quasiplasticity refers to the capability of SMAs to give plastic responds if exposed to compression or tension under θ_{tr}. Here the twinned martensite is the natural configuration of the material, and during the deformation only the twinning interfaces change that is accompanied by no movement of dislocations that would cause irreversible changes. When the transformation is finished the detwinned martensite responds elastically both on further loading or unloading.

The thorough description of these phenomena and their applications may be found in [44, 65, 68], among others.

Shape-memory alloys are highly biocompatible what makes them applicable for many different medical purposes, such as orthodontic wires, cardiovascular stents. For industrial applications different pipes, wires, special connectors and linking elements, etc. are produced to take advantage of their great flexibility, their nonlinear response to stress, or ability to absorb/release significant energy on loading/unloading. Moreover, shape-memory alloys belong to the group of so-called smart or intelligent materials as they both detect the changes in the environment, such as temperature or stress, and also react to them through crystallographic changes in their atomic lattice. On one hand, this feature makes them highly reliable, e.g. in extreme environments where human presence is impossible (just to mention, for example, a recent Mars rover that was also equipped with SMA components), and, on the other hand, their sizes can be significantly reduced without affecting their functionality, cf. Figure 1.1.3, e.g. sputter-deposited NiTi thin films in micro-electro-mechanical systems (MEMS) and microrobotics. For an extensive overview of the modern deposition techniques, key engineering characteristics and applications of NiTi thin films we refer to [61].

Shape-memory alloys exhibit significant hysteresis as well in the martensitic phase transformation (e.g., [32]): the transformation temperature θ_{tr} depends on the direction of the transformation. But hysteresis occurs also in superelasticity: detwinning begins at higher stress than the the reverse transformation. The same applies for the quasiplastic regime as well. In [1] they found that the microstructure evolution of a specimen with exactly two martensitic variants present exhibited a rate-independent hysteresis under cyclic loading. This means that the area under the hysteresis loop does not depend on the rate of loading and is present also at low velocities.

Note that our simplifying assumption of one specific transformation temperature θ_{tr} – above which in a stress-free configuration the austenite is the energetically preferred variant, while below it only the martensite – shall not lead to wrong qualitative results. Under this we will understand the temperature when the austenite and martensite are energetically in equilibrium.

Another peculiarity of the martensitic phase transformation is its activated character – it starts after the external stress exceeds a certain threshold and then completes almost without any further stress increment – that is not captured in theories dealing with the microscopic description of SMAs [2, 69] which predict a linear kinetic relation between the rate of transformation and the applied stress. The stick-slip behaviour can then be recovered through a wiggly energy landscape [1, 20] that pins the phase boundaries, or under hyperelastic assumptions the dissipation (pseudo)potential is supposed to be non-smooth at the origin, cf. [18, 53] among others. We shall also follow this latter path.

Some other characteristics, such as acoustic emission [31, 35] or stress drop at the onset of the stress plateau in the stress–strain curve [37], remain, however, beyond the scope of this work.

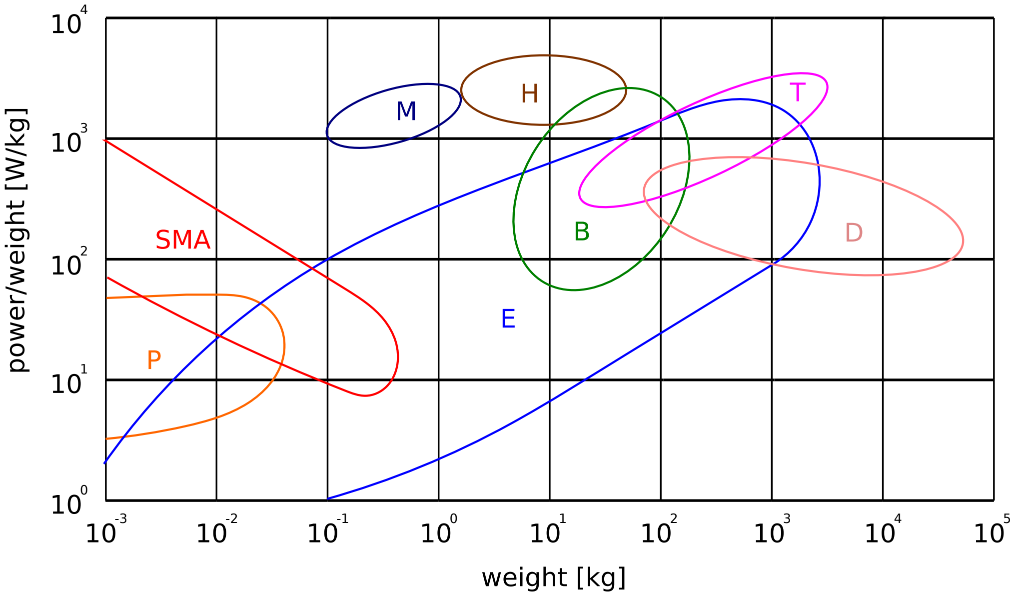

Figure 1.1.3: Power–weight ratio for different types of actuators

Legend for Figure 1.1.3: P – piezoelectric transducers, E – electromotors, M – modeller motors, H – hydraulic motors, B – piston gas-engines, D – piston diesel-engines, T – internal-combustion turbines, SMA – shape-memory alloy actuators (in accordance with [81]).

Biggest disadvantage of shape-memory alloys is their high price and lower heat conductivity. That is where ferromagnetic shape-memory alloys, shape-memory polymers and shape-memory composites come into consideration, cf. [12, 70].

1.2 Atomistic description of SMAs

Modelling of shape-memory alloys can be elaborated on different length scales that is turn involve different phenomenologies and different physical principles. Vaguely speaking, the main scales are the following:

1. The atomistic scale, where molecular dynamics plays the crucial role and interatomic relations are investigated, cf. [73, 74] for advances in related mathematical analysis. Successful experiments on nanoscopic specimen have also been carried out [33, 36].

2. On the microscopic scale one already ascends to a continuum-mechanical description to address single-crystal specimen of sizes of order 100μm. Here one usually accounts for a complete description of the underlying microscopic structure and consideres interfacial effects between variants / phases, cf. [34, 23] among others.

3. The mesoscopic description "zooms further out"(specimen of mm- or cm-size) and utilizes the so-called (gradient) Young measures to associate certain averaged quantities to material points.

4. A macroscopic scale is used to model polycrystalline specimen, the theories being still rather phenomenological and parameter fitting is often applied to match with experimental data. The state of the material is usually described through specific (independent) internal variables, such as the vector of volume fractions of the martensitic variants, or the transformation strain.

On the atomistic scale SMAs can be described as a three-dimensional Bravais lattice $\mathcal{L}$ of infinite number of points generated by translation of a single atom $\mathfrak{o} \in \mathbb{R}^3$ through three linearly independent vectors – the so-called lattice vectors – $\{v_1, v_2, v_3\}$

$$\mathcal{L}(v_i, \mathfrak{o}) = \left\{ x \in \mathbb{R}^3 \colon x = \mathfrak{o} + \sum_{i=1}^{3} \mu^i v_i, \ \mu^i \in \mathbb{Z} \right\}.$$

If we denote by $\{v_1^a, v_2^a, v_3^a\}$ the lattice vectors of the austenite phase and by $\{v_1^m, v_2^m, v_3^m\}$ the lattice vectors of the martensite, then there exists a linear transformation (recall that the martensitic phase transformation is diffusionless), represented by the so-called Bain (or transformation or distortion) matrix U, such that

$$v_i^m = U v_i^a,$$

which is intimately related to the symmetries of the two phases. The set of transformations $\mathcal{G}(v_i)$ mapping the lattice back to itself is called the symmetry group of the lattice, and it is not hard to see that

$$\mathcal{G}(v_i) = \{Q \in O(3) \colon \mathcal{L}(Qv_i) = \mathcal{L}(v_i)\},$$

where $O(d) = \{Q \in \mathbb{R}^{d\times d} \colon Q^\top Q = QQ^\top = I\}$ denotes the orthogonal group, I standing for the $d \times d$ identity matrix. This set includes both shears, rotations, and reflections, as well, but due to the small relative motions of the atoms during the martensitic transformation – as explained previously – shears are relevant rather for plasticity and slip theories. Therefore a smaller, more natural, group is introduced containing the orientation-preserving rotations mapping the lattice onto itself, the so-called point group $\mathcal{P}(v_i)$,

$$\mathcal{P}(v_i) = \{Q \in SO(3) \colon \mathcal{L}(Qv_i) = \mathcal{L}(v_i)\},$$

where $SO(d) = \{Q \in \mathbb{R}^{d\times d} \colon Q^\top Q = QQ^\top = I, \det Q = 1\}$ is called the special orthogonal group.

It can be shown that $\mathcal{P}(v_i)$ is independent of the lattice itself or the chosen lattice vectors, and that there exist in the three-dimensional case 11 distinct point groups, dividable into 7 symmetry types: cubic, tetragonal, hexagonal, monoclinic, triclinic, orthorombic, and rhombohedral lattices. For example, the point group of the cubic lattice, cf. Figure 1.2.1, contains 24 rotations, while the point group of the tetragonal one 8 rotations.

Now, if we denote $\mathcal{P}_a$ the point group of the austenite and $\mathcal{P}_m$ the point group of the martensite such that $\mathcal{P}_m \subset \mathcal{P}_a$, then one can show that the total number M of different martensitic variants is equal to the ration of the number of elements of these sets, namely

$$M = \frac{|\mathcal{P}_a|}{|\mathcal{P}_m|}.$$

This means that in the case of, for example, a cubic-to-tetragonal phase transformation there is $M = 24/8 = 3$, cf. Figure 1.2.1.

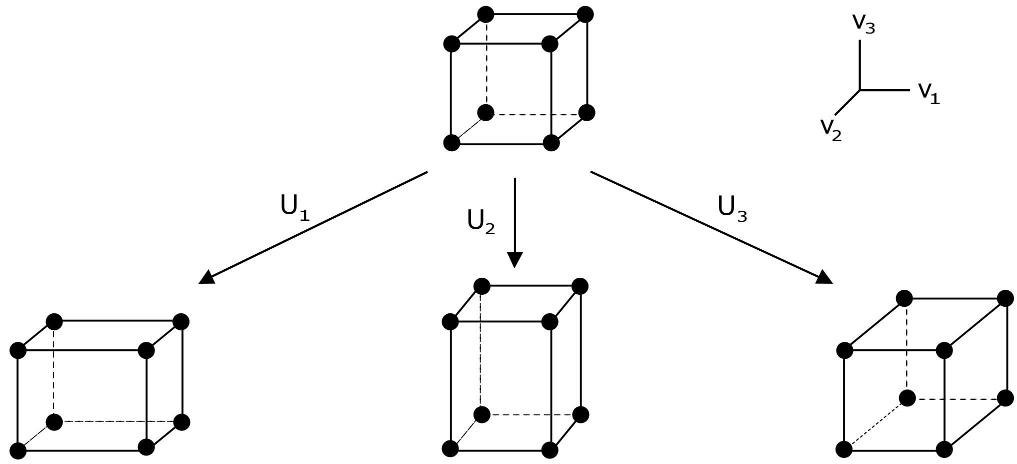

Figure 1.2.1: Different variants of the cubic-to-tetragonal phase transformation

So far we have only discussed the atomic description of SMAs from a crystallographic point of view. To conduct macroscopic experiments or feasible computer simulations, the derivation of a continuum model is desirable. The so-called Cauchy–Born hypothesis (cf. [21]) provides the link between the atomistic and continuum theories. Having a reference domain $\Omega \subset \mathbb{R}^3$, it assumes the following:

1. At each point $x \in \Omega$ of the reference domain there exists a Bravais lattice with lattice vectors $v_i^R(x)$.

2. If Ω is deformed through $y\colon \Omega \to \mathbb{R}^3$, then there exists a Bravais lattice also at $y(x)$ of the actual configuration with lattice vectors $v_i(x)$.

3. (Cauchy–Born hypothesis) The lattice vectors deform according to the deformation gradient, namely
$$v_i(x) = \nabla y(x) v_i^R(x) \quad \forall x \in \Omega.$$

Let us note that however intuitive the Cauchy–Born hypothesis is, Friesecke and Theil [43] have shown that although in some cases it may be regarded as a theorem, there are simple counterexamples, when it fails to hold.

The most important consequence of the Cauchy–Born hypothesis for us here is that instead of Bravais lattices we are entitled to describe SMA configurations by deformation gradients.

1.3 Static micro-scale continuum modelling

First, let us fix some notation. We will consider a specimen in a reference configuration (in this work it shall exclusively be the stress-free austenite phase) occupying a domain $\Omega \subset \mathbb{R}^3$, an admissible deformation as an injective and sufficiently smooth mapping $y(t)\colon \Omega \to \mathbb{R}^3$ over a finite time interval $[0, T]$, $T \in \mathbb{R}^+$, such that $\det \nabla y(t, x) > 0$, for every $x \in \Omega$ and $t \in [0, T]$, and the temperature $\theta\colon \Omega \to \mathbb{R}$.

As usual in continuum thermodynamics (cf. [78]), the equilibrium states of the material are described the as minimizers of a certain thermodynamic energy (potential), that is, the Gibbs free energy $\mathcal{G}(t, y, \theta)$ (in case of vanishing external forces the Helmholtz free energy). In general, the following natural conditions (1.–2.) and constitutive assumptions on the density of this free energy are made.

1. Frame-indifference, that is, the energy of a rigidly rotated material stays the same.

2. Material symmetry, that is, the energy of the material does not depend on the choice of the lattice vectors (in terms of the continuum framework, the deformations from the point group of symmetry do not change the free energy).

3. The order parameter of the free energy is the deformation gradient which identifies the different phases.

4. Single-variant phases minimize the free energy, i.e., they are stable.

5. During a thermally induced phase transition the material transforms from a low-temperature stable austenite to a high-temperature stable martensite. At the transformation temperature θ_{tr} both phases are energetically equivalent.

6. The energy density blows up for deformations approaching a singular one (i.e., one with vanishing determinant of the strain).

Some remarks are at place here. Firstly, geometrically linear models – or infinitezimal strains, that is, instead of the deformation gradient only its symmetric part is considered – have been proposed, but these can lead to significant errors, cf. [19] and the references therein, and when later applying the theory to thin films, they can deform by undergoing large rotations, e.g. by forming tents and tunnels [23].

Secondly, the last condition, although natural to presume, is in conflict with the usual p-growth assumption on the free energy density in existence theorems for the relaxed variational problems, and does not seem to be a mere technicality to deal with. We shall discuss the topic later on in larger extent.

There are many different ways how to construct a free energy that is able to describe the behaviour of SMAs. One of the first approaches was to consider phenomenological theories of Landau, Devonshire or Ginzburg-Landau type. The free energy $f(e, \theta)$, e being an order parameter and θ the temperature, was assumed to be analytical in e, the expansion of which into a power series with respect to e yielded partial results enlightening some aspects of the martensitic transformation as well, cf. the works of Falk and Konopka [38, 39]. This polynomial free energy approach inspired also the more recent work of Zimmer [84].

We shall follows the path of Ball and James [6, 7] who proposed a Helmholtz free energy density of multi-well structure. We take the Gibbs free energy $\mathcal{G}$ that is the Helmholtz free energy augmented with the external loads

$$\mathcal{G}(y, \nabla y, \theta) = \int_\Omega \varphi(\nabla y(x), \theta(x))\,\mathrm{d}x - \int_\Omega f(x)\cdot y(x)\,\mathrm{d}x - \int_{\Gamma_N} g(x)\cdot y(x)\,\mathrm{d}S, \quad (1.3.1)$$

where $\Gamma_N \subset \partial\Omega$ is the boundary part where the prescribed external surface force g acts, f is then a prescribed external volume force, and we fix the specimen on the Dirichlet boundary part $\Gamma_D = \partial\Omega \setminus \Gamma_N$ (up to a zero-measure set) of non-vanishing 2-dimensional measure. The stored energy density φ then satisfies

1. frame indifference

$$\varphi(QF, \theta) = \varphi(F, \theta) \quad \forall Q \in SO(3);$$

2. material symmetry

$$\varphi(FR, \theta) = \varphi(F, \theta) \quad \forall R \in \mathcal{P}_a, ;$$

3. temperature dependence

$$\begin{aligned} 0 = \varphi(\mathcal{I}, \theta) &< \varphi(F, \theta), & \theta &> \theta_{\mathrm{tr}}, \\ 0 = \varphi(\mathcal{I}, \theta) = \varphi(\mathcal{U}, \theta) + \delta(\theta) &< \varphi(F, \theta), & \theta &= \theta_{\mathrm{tr}}, \\ 0 = \varphi(\mathcal{U}, \theta) + \delta(\theta) &< \varphi(F, \theta), & \theta &< \theta_{\mathrm{tr}}, \end{aligned}$$

for every $\mathcal{I} \in \mathcal{A}$ and $\mathcal{U} \in \mathcal{M}$, where $\delta(\theta)$ is an offset, and $\mathcal{A}$ and $\mathcal{M}$ represent the sets of the austenite and martensite wells, respectively, namely

$$\begin{aligned} \mathcal{A} &= \{Q : \; Q \in SO(3)\} \equiv SO(3)I, \\ \mathcal{M} &= \mathcal{M}_1 \cup \mathcal{M}_2 \cup \cdots \cup \mathcal{M}_M \equiv \bigcup_{i=1}^{M} SO(3)U_i. \end{aligned}$$

Note that due to material frame indifference we can consider the Bain matrices U_i symmetric (if they are not, thanks to the polar decomposition theorem they can be decomposed into a symmetric, positive-definite matrix and a rotation – recall that any admissible deformation satisfies $\det \nabla y > 0$).

We will use the minimum type multi-well energy density, cf. [53]

$$\varphi(F, \theta) = \min_{m=0,\ldots,M} \varphi_m, \quad (1.3.2)$$

where

$$\begin{aligned} \varphi(F, \theta) &= \frac{1}{2} \sum_{ijkl} \epsilon^m_{ij} C^m_{ijkl} \epsilon^m_{kl} + c^m_V \theta_{\mathrm{tr}} \ln\left(\frac{\theta}{\theta_{\mathrm{tr}}}\right), \\ \epsilon^m &= \frac{F^\top F - U_m^\top U_m}{2}, \end{aligned}$$

C^m being the tensor of elastic moduli and c_V^m the specific heat capacity.

One of the easiest models to deal with are the isothermal static cases. On the microscopic scale one might include an interfacial-energy term to account for another length scale concerning the interfaces between the variants. More precisely,

$$\begin{cases} \text{minimize} & \mathcal{G}(y, \nabla y, \theta_{\text{tr}}) + \mathcal{E}_{\text{interface}}(\nabla^2 y) \\ \text{subject to} & y \in W^{2,2}(\Omega; \mathbb{R}^3) \\ & y = id \text{ on } \Gamma_D, \end{cases} \tag{1.3.3}$$

where $\mathcal{G}$ is as defined in (1.3.1) and (1.3.2). The interfacial energy involves the second derivatives of the deformation y, and is usually of the form $\mathcal{E}_{\text{interface}}(\nabla^2 y) = \varepsilon \|\nabla^2 y\|^2_{L^2(\Omega;\mathbb{R}^{3\times3\times3})}$, cf. [23], or $\varepsilon\|\triangle y\|^2_{L^2(\Omega;\mathbb{R}^{3\times3})}$, see [22], that differs from the first one only by a null-Lagrangian and penalizing bending as well, for some fixed $\varepsilon > 0$. Another way to incorporate interfacial energy can be found, e.g., in [80].

As the interfacial energy introduces from the mathematical perspective a compactifying effect, the existence of a minimizer $\bar{y}$ to (1.3.3) can be shown through the well-established direct method of the calculus of variations, see [25] for the details.

1.4 Static modelling on mesoscopic scale – quasiconvexification

When neglecting interfacial effect, for a more involved limit passage $\varepsilon \to 0_+$ we refer to [77], one obtains the mesoscopic model

$$\begin{cases} \text{minimize} & \mathcal{G}(y, \nabla y, \theta_{\text{tr}}) \\ \text{subject to} & y \in W^{1,p}_{\Gamma_D}(\Omega; \mathbb{R}^3), \end{cases} \tag{1.4.1}$$

where $W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^3) = \{v \in W^{1,p}(\Omega;\mathbb{R}^3) \colon v = id \text{ on } \Gamma_D\}$, that allows for infinitely fine oscillations in the deformation gradient for microstructure formation. Mathematically, the total energy is not weakly lower semicontinuous, therefore the existence of a classical Sobolev minimizer to (1.4.1) cannot be guaranteed.

This problem is usually resolved by two so-called relaxation methods. The heart of the quasiconvexification is in replacing the energy density φ (1.3.2) by its quasiconvex envelope

$$Q\varphi := \sup\{\Psi \le \varphi : \ \Psi \text{ quasiconvex}\}, \tag{1.4.2}$$

suppressing the temperature dependence. Recall that a function $g \colon \mathbb{R}^{m\times n} \to \mathbb{R}$ is called quasiconvex, if for any $A \in \mathbb{R}^{m\times n}$ and any $\phi \in C_0^\infty(\Omega;\mathbb{R}^m)$ it holds that

$$g(A) \le \frac{1}{|\Omega|}\int_\Omega g(A + \nabla\phi(x))\,\mathrm{d}x, \tag{1.4.3}$$

where $\Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain and $|\Omega|$ denotes the n-dimensional Lebesgue measure of the set Ω. It can be shown that the property of quasiconvexity is independent of the particular domain Ω; cf. [25].

Now, the relaxed problem reads as

$$\begin{cases} \text{minimize} & \mathcal{G}_Q(y, \nabla y, \theta_{\mathrm{tr}}) \\ \text{subject to} & y \in W^{1,p}_{\Gamma_D}(\Omega; \mathbb{R}^3), \end{cases} \tag{1.4.4}$$

where

$$\mathcal{G}_Q(y, \nabla y, \theta_{\mathrm{tr}}) := \int_\Omega Q\varphi(\nabla y(x), \theta_{\mathrm{tr}})\,\mathrm{d}x - \int_\Omega f(x) \cdot y(x)\,\mathrm{d}x - \int_{\Gamma_N} g(x) \cdot y(x)\,\mathrm{d}S.$$

Then, the relaxation theorem (due to Dacorogna; cf. [25]) states that under the growth condition

$$c(|s|^p - 1) \le \varphi(s) \le C(|s|^p + 1), \text{ for some real } 0 < c \le C, \tag{1.4.5}$$

the following holds

(i)
$$\inf_{y \in W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^3)} \mathcal{G}(y, \nabla y, \theta_{\mathrm{tr}}) = \min_{y \in W^{1,p}_{\Gamma_D}(\Omega;\mathbb{R}^3)} \mathcal{G}_Q(y, \nabla y, \theta_{\mathrm{tr}}); \tag{1.4.6}$$

(ii) to each solution y^* of the relaxed problem (1.4.4) there exists a minimizing sequence of the initial problem (1.4.1) that converges to y^* weakly in $W^{1,p}(\Omega; \mathbb{R}^3)$;

(iii) any infimizing sequence of the initial problem (1.4.1) converges weakly in $W^{1,p}(\Omega; \mathbb{R}^3)$ to a minimizer of the relaxed problem (1.4.4).

Note that the relaxed functional $\mathcal{G}_Q$ inherits coercivity, namely the p-growth property applies for $Q\varphi$ as well, see (1.4.5).

Quasiconvexification is a successful tool to overcome the non-existence of minimizers to coercive functional that are not weakly sequentially lower semicontinuous on reflexive Sobolev spaces. Its intention is to alter the functional in a way that preserves the original infimum and is attained by the original infimizing sequences. Information about the oscillations of the infimizing sequences is lost, however.

Another tool (called Young measures) ensures existence of a minimizer, while conserving information about the oscillatory behaviour of the corresponding sequence, was introduced by L. C. Young [83] – originally in the context of optimal control theory. Since then it has been successfully applied not only in problems of non-linear elasticity, but also, e.g., in fluid dynamics (their generalization, the so-called DiPerna-Majda measures, was developed to analyse weak solutions of incompressible fluid dynamics equations [28].

1.5 Static modelling on mesoscopic scale – Young measures

First, let us recall some notation and facts from functional analysis. We denote by $C_0(\Omega; \mathbb{R}^{m\times n}) \simeq \overline{C_c(\Omega; \mathbb{R}^{m\times n})}$ the set of all continuous functions with values in $\mathbb{R}^{m\times n}$ vanishing at infinity, that is the closure of the set of all compactly supported continuous functions, $\Omega \subset \mathbb{R}^d$ measurable with finite measure. Through the Riesz Theorem, its dual space $C_0(\Omega;\mathbb{R}^{m\times n})^*$ is isomorphic to the space of all regular countably additive measures $\mathrm{rca}(\mathbb{R}^{m\times n})$ augmented with the total variation norm.

Then $L^\infty_w(\Omega;\mathrm{rca}(\mathbb{R}^{m\times n})) \simeq L^1(\Omega;C_0(\mathbb{R}^{m\times n}))^*$ is the set of all essentially bounded weakly-$\star$ measurable mappings $x \mapsto \mu_x\colon \Omega \to \mathrm{rca}(\Omega^{m\times n})$, meaning that the maps $x \mapsto \langle \mu_x, v\rangle = \int_{R^{m\times n}} v(A)\,\mathrm{d}\mu_x(A)$ are Lebesgue measurable. To keep the text as lucid as possible, we introduce also the so-called momentum operator $\bullet\colon C_0(\mathbb{R}^{m\times n}) \times L^\infty_w(\Omega;\mathrm{rca}(\mathbb{R}^{m\times n})) \to L^\infty(\Omega)$ for a family of parametric measures $\mu = \{\mu_x\}_{x\in\Omega}$ as

$$(f \bullet \mu)(x) := \int_{\mathbb{R}^{m\times n}} f(A)\,\mathrm{d}\mu_x(A), \tag{1.5.1}$$

i.e., the x-dependent duality pairing $\langle \mu_x, f\rangle$.

We shall utilize also the space of continuous functions with sub-p growth

$$C_p(\mathbb{R}^{m\times n}) = \left\{ v \in C(\mathbb{R}^{m\times n})\colon v(s) = o(|s|^p) \text{ for } |s| \to \infty \right\}.$$

Before defining Young measures, let us state the main theorem describing their essential property, i.e., the ability of capturing the limits for all continuous functions with appropriate growth. The second part is the generalization for L^p-bounded sequences by [72].

Theorem 1.5.1 (Fundamental theorem of Young measures)**.**

(i) Let $\{u_k\}_{k\in\mathbb{N}} \subset L^\infty(\Omega;\mathbb{R}^{m\times n})$ a bounded sequence, more precisely, $u_k(x) \in K$ for some compact $K \subset \mathbb{R}^{m\times n}$, for a.e. $x \in \Omega$ and all $k \in \mathbb{N}$.

Then there exists a (not relabelled) subsequence of $\{u_k\}_{k\in\mathbb{N}}$ and a parametrized probability measure $\nu = \{\nu_x\}_{x\in\Omega} \in L^\infty_w(\Omega;\mathrm{rca}(\mathbb{R}^{m\times n}))$ such that

$$f \circ u_k \overset{*}{\rightharpoonup} f \bullet \nu \text{ in } L^\infty(\Omega) \quad \forall f \in C_0(\mathbb{R}^{m\times n}). \tag{1.5.2}$$

Moreover, $\operatorname{supp} \nu_x \subset K$ *for a.e. $x \in \Omega$.*

(ii) Let $\{u_k\}_{k\in\mathbb{N}} \subset L^p(\Omega;\mathbb{R}^{m\times n})$ a bounded sequence for some $1 < p < \infty$. Then there exists a (not relabelled) subsequence of $\{u_k\}_{k\in\mathbb{N}}$ and a parametrized probability measure $\nu = \{\nu_x\}_{x\in\Omega} \in L^\infty_w(\Omega;\mathrm{rca}(\mathbb{R}^{m\times n}))$ such that

$$f \circ u_k \rightharpoonup f \bullet \nu \text{ in } L^1(\Omega) \quad \forall f \in C_p(\mathbb{R}^{m\times n}). \tag{1.5.3}$$

Note that (1.5.2) holds for all continuous f and that (1.5.3) holds for $p = 1$, as well [25].

Now, let us define the set of Young measures and L^p-Young measures, respectively, as parametrized measures that are generated in this way, that is, in accord with Theorem 1.5.1 (i) and (ii), respectively.

Definition 1.5.1. Let $1 < p < \infty$, $\Omega \subset \mathbb{R}^d$ a bounded domain. Then we define the set of Young measures as

$$\begin{aligned}\mathcal{Y}^\infty(\Omega;\mathbb{R}^{m\times n}) := \Big\{ \nu \in L^\infty_w(\Omega;\mathrm{rca}(\mathbb{R}^{m\times n}))\colon \exists \{u_k\}_{k\in\mathbb{N}} \subset L^\infty(\Omega;\mathbb{R}^{m\times n}) \text{ s.t.}\\ f \circ u_k \overset{*}{\rightharpoonup} f \bullet \nu \text{ in } L^\infty(\Omega) \text{ for all } f \in C_0(\mathbb{R}^{m\times n}) \Big\},\end{aligned}$$

and the set of L^p-Young measures as

$$\mathcal{Y}^p(\Omega;\mathbb{R}^{m\times n}) := \big\{\nu \in L^\infty_w(\Omega;\mathrm{rca}(\mathbb{R}^{m\times n}))\colon \exists\{u_k\}_{k\in\mathbb{N}} \subset L^p(\Omega;\mathbb{R}^{m\times n}) \text{ s.t. } f\circ u_k \rightharpoonup f\bullet\nu \text{ in } L^1(\Omega) \text{ for all } f\in C_p(\mathbb{R}^{m\times n})\big\}\,.$$

We call ν the associated Young measure to the generating sequence $\{u_k\}$.

Although having convergence in (1.5.2) and (1.5.3) for some particular integrands f, it can be shown that Young measures preserve weak lower semicontinuity for much more general functions f, cf. [40, Theorem 8.6(i)].

Proposition 1.5.1. *Let the bounded sequence $\{u_k\}_{k\in\mathbb{N}} \subset L^p(\Omega;\mathbb{R}^{m\times n})$ generate $\nu \in \mathcal{Y}^p(\Omega;\mathbb{R}^{m\times n})$, $1<p<\infty$. Let $f\colon \mathbb{R}^{m\times n}\to[-\infty,+\infty]$ be a normal integrand such that its negative part $\{f^-(u_k)\}_{k\in\mathbb{N}}$ is equi-integrable. Then*

$$\int_\Omega f\bullet\nu\,dx \le \liminf_{k\to\infty}\int_\Omega f(u_k(x))\,dx.$$

Lastly, let us note that an explicit characterization of Young measures is also useful, when one does not have to rely on generating sequences to identify these particular parametrized measures. The proof of the first part can be found, e.g., in [63] or [67], the second part was proved by Kružík and Roubíček in [55].

Proposition 1.5.2. *Let $1<p<\infty$ and $\nu\in L^\infty_w(\Omega;\mathrm{rca}(\mathbb{R}^{m\times n}))$. Then*

(i) $\nu\in\mathcal{Y}^\infty(\Omega;\mathbb{R}^{m\times n})$ *if and only if there exists some compact $K\subset\mathbb{R}^{m\times n}$ such that* $\operatorname{supp}\nu_x\subset K$ *for a.e. $x\in\Omega$.*

(ii) $\nu\in\mathcal{Y}^p(\Omega;\mathbb{R}^{m\times n})$ *if and only if* $\int_\Omega|\cdot|^p\bullet\nu\,dx$.

In what follows we examine some subsets of Young measures that play a significant role – among others – in relaxation of variational elasticity problems.

One of the most important subsets of Young measures is the one which can be generated by gradients.

Definition 1.5.2. Let $\Omega\subset\mathbb{R}^d$ be a bounded open domain, $1<p<\infty$. Then we define the set of gradient Young measures as

$$\mathcal{G}^\infty(\Omega;\mathbb{R}^{n\times d}) := \big\{\nu\in\mathcal{Y}^\infty\colon \exists\{u_k\}_{k\in\mathbb{N}}\subset W^{1,\infty}(\Omega;\mathbb{R}^n) \text{ bounded such that } \{\nabla u_k\}_{k\in\mathbb{N}} \text{ generates } \nu\big\}\,,$$

and the set of L^p-gradient Young measures as

$$\mathcal{G}^p(\Omega;\mathbb{R}^{n\times d}) := \big\{\nu\in\mathcal{Y}^p\colon \exists\{u_k\}_{k\in\mathbb{N}}\subset W^{1,p}(\Omega;\mathbb{R}^n) \text{ bounded such that } \{\nabla u_k\}_{k\in\mathbb{N}} \text{ generates } \nu\big\}\,,$$

The explicit characterization of $\mathcal{G}^\infty$ and $\mathcal{G}^p$ is due to Kinderlehrer and Pedregal [46, 47]. In short, they showed that a parametrized measure $\nu\in L^\infty_w(\Omega;\mathrm{rca}(\mathbb{R}^{n\times d}))$ is a gradient Young measure if and only if (i) it is a Young measure, (ii) its barycentre corresponds to a Sobolev-function gradient, and (iii) it satisfies a Jensen-type inequality for certain quasiconvex functions.

Theorem 1.5.2 (Gradient Young measures, cf. [46]). *Let the assumptions of Definition 1.5.2 hold, and let $\nu \in L^\infty_w(\Omega; \mathrm{rca}(\mathbb{R}^{n\times d}))$. Then $\nu \in \mathcal{G}^\infty(\Omega; \mathbb{R}^{n\times d})$ if and only if the following conditions hold:*

(i) $\operatorname{supp} \nu_x \subset K$ *for a.e.* $x \in \Omega$ *for some* $K \subset \mathbb{R}^{n\times d}$*;*

(ii) $\nabla u = id \bullet \nu$ *a.e. in* Ω *for some* $u \in W^{1,\infty}(\Omega; \mathbb{R}^n)$*;*

(iii) $f(\nabla u) \le f \bullet \nu$ *a.e. in* Ω *for all* f *continuous, quasiconvex, bounded from below.*

A similar characterization can be shown for the finite exponent $1 < p < \infty$ (in fact, it holds for $p = 1$ as well).

Theorem 1.5.3 (L^p-gradient Young measures, cf. [47]). *Let the assumptions of Definition 1.5.2 hold, and let $\nu \in L^\infty_w(\Omega; \mathrm{rca}(\mathbb{R}^{n\times d}))$, $1 < p < \infty$. Then $\nu \in \mathcal{G}^p(\Omega; \mathbb{R}^{n\times d})$ if and only if the following conditions hold:*

(i) $\int_\Omega |\cdot|^p \bullet \nu \, dx < \infty$*;*

(ii) $\nabla u = id \bullet \nu$ *a.e. in* Ω *for some* $u \in W^{1,p}(\Omega; \mathbb{R}^n)$*;*

(iii) $f(\nabla u) \le f \bullet \nu$ *a.e. in* Ω *for all* f *continuous, quasiconvex, bounded from below such that* $|f|(s) \le C(1 + |s|^p)$*.*

At last, the following relaxation of our initial mesoscopic problem (1.4.1) can be proven, cf. [25], for example.

$$\begin{cases} \text{minimize} & \mathcal{G}_{\mathrm{YM}}(y, \nu, \theta_{\mathrm{tr}}) \\ \text{subject to} & y \in W^{1,p}(\Omega; \mathbb{R}^3), \\ & \nu \in \mathcal{G}^p_{\Gamma_D}(\Omega; \mathbb{R}^{3\times 3}), \\ & \nabla y = id \bullet \nu \text{ a.e. in } \Omega, \end{cases} \tag{1.5.4}$$

where the relaxed functional $\mathcal{G}_{\mathrm{YM}}$ reads as

$$\mathcal{G}_{\mathrm{YM}}(y, \nu, \theta_{\mathrm{tr}}) := \int_\Omega \varphi \bullet \nu_x \, \mathrm{d}x - \int_\Omega f(x) \cdot y(x) \, \mathrm{d}x - \int_{\Gamma_N} g(x) \cdot y(x) \, \mathrm{d}S, \tag{1.5.5}$$

and every Young measure $\mu \in \mathcal{G}^p_{\Gamma_D}(\Omega; \mathbb{R}^{3\times 3})$ admits a generating sequence contained in $W^{1,p}(\Omega; \mathbb{R}^{3\times 3})$.

1.6 Evolutionary SMA models with constant temperature

Static models provide valuable information about material stable states under different external loads. However, to capture for example the hysteretic behaviour of shape-memory alloys, cf. Figure 1.1.1, one needs to introduce more involved evolutionary models. An interesting phenomenon has been experimentally confirmed, see [75], [76], namely that the final microstructure of the specimen is in fact path-dependent. Therefore one has to take into account dissipation effects during the process of evolution (cf. [64] for a thorough overview).

One of the most popular methods to model shape-memory alloy evolution, as long as energy minimization is concerned, adapts the concept of generalized standard materials, initially developed by Halphen and Nguyen [45]. According to their definition the model of the material behaviour should be defined by two potentials: the energy potential $\varphi(\alpha)$, which should be a function of the state variables α, and a dissipation potential $R(\alpha, \dot{\alpha})$, a convex function of the flux $\dot{\alpha}$, depending perhaps on the state α as well.

In general, one usually chooses R in such a way that the following inclusion holds

$$\partial_{\dot{\alpha}} R(\alpha, \dot{\alpha}) \ni A, \tag{1.6.1}$$

where A represents the generalized forces. This ensures then thermodynamic consistency (non-negativity of the dissipation rate $\mathcal{D}$), as

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

where we exploited the convexity of R.

In light of this latter description, the evolution of the specimen is governed by the following doubly-non-linear problem

$$\partial R(\dot{\alpha}) + \mathcal{G}'_\alpha(\alpha) \ni 0, \tag{1.6.2}$$

if sufficient smoothness is available for the Gibbs potential $\mathcal{G}$. Note that (1.6.2) incorporates both the balance of momentum and that flow rule which governs the evolution of the vector of the so-called internal parameters χ, where $\alpha = (\nabla y, \chi)$.

Lastly, let us remark that (1.6.2) is related to Levitas' realizability principle cf. [60], namely that the phase transformation occurs as soon as the energy gain of a particular state (transformation) reaches the level of the dissipated energy.

When ascending to a mesoscopic description, i.e., vaguely speaking, replacing the Gibbs energy $\mathcal{G}$ by $\mathcal{G}_{\text{YM}}$ from (1.5.5), the inclusion (1.6.2) becomes rather formal due to the lack of smoothness (this stems from the constraint that the Young measure has to be generated by gradients, cf. [53]).

A correct definition of a weak solution to such problems – in the sense that under sufficient regularity hypothesis it is a solution to (1.6.2) as well – has been introduced by Mielke and Theil [58, 59, 60], called an energetic solution. Let us sketch the basic philosophy of this concept as it shall play a significant role later during the analysis of a thermodynamically coupled thin-film SMA model in Chapter 2 as well.

We follow [53] to introduce a mesoscopic rate-independent evolution model for shape-memory alloys and its energetic solution. In order to do so, let us consider the respective energies

$$\mathcal{G}_{\text{evol}}(t, q) := \mathcal{G}_{\text{evol}}(t, y, \mu, \lambda) = \int_\Omega \varphi \bullet \mu_x - f(t) \cdot y \,\mathrm{d}x - \int_{\Gamma_N} g(t) \cdot y \,\mathrm{d}S + \varrho \|\lambda\|^r_{\alpha,r}, \tag{1.6.3}$$

where $\varrho > 0$ is some small parameter, $\|\lambda\|^r_{\alpha,r}$ denotes the norm of the internal parameter, the so-called vector of volume fractions here, in the Sobolev–Slobodeckii space $W^{\alpha,r}(\Omega; \mathbb{R}^{M+1})$, $0 < \alpha < 1$ (this term is included mainly for its compactifying effect for the embedding $W^{\alpha,r}(\Omega; \mathbb{R}^{M+1}) \hookrightarrow L^1(\Omega; \mathbb{R}^{M+1})$). The vector of (mesoscopic) volume fractions is defined as

$$\lambda(x) = \mathcal{L} \bullet \nu_x, \quad \text{where } \mathcal{L} \colon \mathbb{R}^{3\times 3} \to \{\zeta \in \mathbb{R}^{M+1} \colon \zeta_i \geq 0,\, i = 0, \ldots, M,\, \textstyle\sum \zeta_i = 1\}$$

is a continuous function identifying the different phases and variants, i.e. $L_i(F) = 1$ whenever F is in the vicinity of the i-th well $SO(3)U_i$. The dissipation potential is taken in the following form

$$R_{\text{evol}}(\dot{q}) := \int_\Omega \sum_{i=0}^{M} \gamma_i |\dot{\lambda}_i| \,\mathrm{d}x, \tag{1.6.4}$$

where $0 < \gamma_i \ll \gamma_0$, for $i = 1, \dots, M$, reflecting on the fact that the biggest contribution to the dissipated energy is through the austenite–martensite transformation.

The doubly-non-linear problem (1.6.2) can now be specified in terms of (1.6.3) and (1.6.4) as

$$\begin{aligned} \partial_\nu \mathcal{G}_{\text{evol}}(t, q(t)) &\ni 0 && \text{in } (0,T)\times\Omega, \\ \partial_{\dot\lambda} R_{\text{evol}}(\dot{q}) + [\mathcal{G}_{\text{evol}}]'_\lambda (t, q(t)) &\ni 0 && \text{in } (0,T)\times\Omega, \\ \nabla y(x) &= id \bullet \nu_x && \text{for a.e. } x\in\Omega, \\ \lambda(x) &= \mathcal{L} \bullet \nu_x && \text{for a.e. } x\in\Omega, \\ q(0) &= q_0 && \text{in } \Omega, \\ y(x) &= y_D(x) && \text{on } [0,T]\times\Gamma_D, \end{aligned} \tag{1.6.5}$$

where $\Gamma_D \subset \partial\Omega$, such that $|\Gamma_D|_2 > 0$.

Definition 1.6.1 (Energetic solution)**.** A process $q\colon [0,T] \to Q$, where

$$Q := \big\{(y,\nu,\lambda) \in W^{1,p}(\Omega;\mathbb{R}^m) \times \mathcal{G}^p(\Omega;\mathbb{R}^{3\times 3}) \times L^1(\Omega;\mathbb{R}^{M+1})\colon \\ \nabla y = id \bullet \nu \text{ and } \lambda = \mathcal{L}\bullet\nu \text{ a.e. in } \Omega,\ y|_{\Gamma_D} = y_D\big\}$$

and y_D is a prescribed load on a Dirichlet boundary $\Gamma_D \subset \partial\Omega$, will be called an energetic solution to the problem (1.6.5), if it satisfies

(i) the initial condition $q(0) = q_0$;

(ii) the static stability condition

$$\mathcal{G}_{\text{evol}}(t, q(t)) \le \mathcal{G}_{\text{evol}}(t, q^\star) + R(q^\star - q(t)),$$

at every time instance $t \in [0,T]$ and for every process $q^\star \in Q$;

(iii) the energy equality

$$\mathcal{G}_{\text{evol}}(t, q(t)) + \mathrm{Var}_{R_{\text{evol}}}(q; s, t) = \mathcal{G}_{\text{evol}}(s, q(s)) + \int_s^t \frac{\partial \mathcal{G}_{\text{evol}}}{\partial\vartheta}(\vartheta, q(\vartheta))\,\mathrm{d}\vartheta,$$

for every $s, t \in [0,T]$.

Here $\mathrm{Var}_{R_{\text{evol}}}(q; s, t)$ stands for the total variation of the process q over the time interval $[s,t]$ with respect to R_{evol}, more precisely

$$\mathrm{Var}_{R_{\text{evol}}}(q; s, t) = \sup\left\{ \sum_{i=1}^{k} R_{\text{evol}}(q(t_i) - q(t_{i-1}))\colon \\ s = t_0 < t_1 < \dots < t_k = t,\ k\in\mathbb{N}, \text{ is a partition of } [s,t] \right\}.$$

Theorem 1.6.1 (see [53]). *Under the following additional assumption on the data:*

$$
\begin{aligned}
&c(|s|^p - 1) \le \varphi(s) \le C(|s|^p + 1) \quad \textit{for some } 0 < c < C < +\infty, \\
&y_D = id, \quad q_0 = (y_0, \nu_0, \lambda_0) \in Q, \\
&f \in W^{1,1}(0,T; L^{p^{*\prime}}(\Omega; \mathbb{R}^3)), \quad g \in W^{1,1}(0,T; L^{p^{\#\prime}}(\Gamma_N; \mathbb{R}^3)),
\end{aligned}
$$

there exists an energetic solution to the doubly-non-linear problem (1.6.5) *in the sense of* (1.6.1).

The proof follows the strategy established in the pioneering works of Mielke, Theil and Levitas [58, 59, 60], however, special care has to be taken of the constraint $\lambda = \mathcal{L} \bullet \nu$. It could destroy the convergence of the volume fractions that is the result of the compactness guaranteed by the non-local ϱ-term in (1.6.3). A work-around is established by introducing the following family of Gibbs' energies that incorporate a relaxation of the aforementioned constraint:

$$
\mathcal{G}^{\epsilon}_{\text{evol}}(t, q(t)) := \mathcal{G}_{\text{evol}}(t, q(t)) + \frac{1}{\epsilon}\|\lambda(t) - \mathcal{L} \bullet \nu\|_{H^{-1}(\Omega;\mathbb{R}^{M+1})}.
$$

The norm of the residuum is computed in $H^{-1}(\Omega;\mathbb{R}^{M+1}) = W^{1,2}_0(\Omega;\mathbb{R}^{M+1})^*$, but in principle any space does the work into which $L^\infty(\Omega;\mathbb{R}^{M+1}) + W^{\alpha,r}(\Omega;\mathbb{R}^{M+1})$ is compactly embedded. This strategy shall be applied also in the thermodynamically coupled cases (for the bulk and thin films, as well). For any details of the proof we refer to [53].

1.7 Evolutionary SMA models with thermal coupling

So far we considered in every model the temperature constant at the so-called transformation temperature. It allowed us to describe equilibrium states that incorporate material microstructure and the evolution of such a microstructure under varying external loads. A fully thermodynamic model devised to capture, e.g., the shape-memory effect also (cf. Figure 1.1.1) has been introduced and thoroughly analysed by Benešová and Roubíček [18], cf. [17] as well that is based upon similar ideas while accounting for additional (thermo)magnetization of certain shape-memory alloys.

To set the problem up, let us take the following energies that include the absolute temperature $\theta\colon [0,T] \to \mathbb{R}^+$ as well in the following form:

$$
\mathcal{G}^{\star}_{\text{therm}}(t, q, \theta) := \mathcal{G})\text{evol}(t, q) + \|\lambda - \mathcal{L} \bullet \nu\|_{H^{-1}} + \int_\Omega \varphi_{\text{therm}}(\theta) + (\theta - \theta_{\text{tr}})\vec{a} \cdot \lambda \,\mathrm{d}x, \tag{1.7.1}
$$

and

$$
R_{\text{therm}}(\dot{q}) := \int_\Omega \frac{\alpha}{q}|\dot{\lambda}|^q + \delta^*_S(\dot{\lambda}) \,\mathrm{d}x. \tag{1.7.2}
$$

This means that we extend the Gibbs energy $\mathcal{G}_{\text{evol}}$ from the previous section by the already described mismatch term (the residuum of the relaxed constraint $\lambda = \mathcal{L} \bullet \nu$) followed by a purely thermal part and the thermo-mechanic coupling between the temperature and the vector of volume fractions, where $\vec{a} \in \mathbb{R}^{M+1}$ such that $a = (0, 0, \dots, -s_{\text{tr}})$, s_{tr} being the specific transformation entropy (the difference between the entropy of the austenite and martensite).

Let us note that the three terms $\int_\Omega \varphi(\nabla y) + \varphi_{\text{therm}}(\theta) + (\theta - \theta_{\text{tr}})\vec{a} \cdot \lambda \,\mathrm{d}x$ can be interpreted as a partial linearisation ansatz of a more general free energy $\int_\Omega \Phi(\nabla y, \lambda, \theta) \,\mathrm{d}x$ while neglecting thermal expansion. This assumption has already appeared in the literature, cf. [39].

The dissipation potential (1.7.2) includes a small $\alpha \ll 1$ rate-dependent dissipation that, on one hand, is physically relevant as argued in [71] that the behaviour of the SMA material becomes rate-dependent for increasing driving forces, on the other hand, mathematically it regularizes λ and makes the analysis feasible. Note that the second term, the Legendre–Fenchel conjugate of the indicator function of a convex set S is a generalization of the previously considered dissipation (1.6.4). Indeed, take the set $\mathcal{H} = \{x \in \mathbb{R}^{M+1} \colon |x_i| \le \gamma_i\}$ for some $\gamma_i \ge 0$, $i = 1, \dots, M+1$, then

$$\delta^*_{\mathcal{H}}(x^*) = \sup_{x \in \mathbb{R}^{M+1}} \{(x^*, x) - \delta_{\mathcal{H}}(x)\} = \sup_{x \in \mathcal{H}} \left\{ \sum_{i=1}^{M+1} x_i^* x_i \right\} = \sum_{i=1}^{M+1} x_i^* \cdot \gamma_i \frac{x_i^*}{|x_i^*|}.$$

The evolution of the temperature is then usually governed by the heat equation, i.e., $c_v(\theta)\dot{\theta} - \operatorname{div} q$ = rate of heat production, where c_v is the specific heat capacity (considered positive) and q the heat flux. However, due to its mathematical advantages we shall introduce the so-called enthalpy $w \colon [0, T] \to \mathbb{R}^+$ through the enthalpy transformation

$$w = \hat{c}_v(\theta) := \int_0^\theta c_v(\vartheta) \,\mathrm{d}\vartheta, \quad \text{denoting the inverse as} \quad \theta = \Theta(w) := \hat{c}_v^{-1}(w). \tag{1.7.3}$$

Furthermore, we apply the Fourier law on the heat flux, namely $q = \mathbb{K}(\lambda, \theta)\nabla\theta$, or in terms of the enthalpy: $q = \mathcal{K}(\lambda, w)\nabla w$, where $\mathcal{K}(\lambda, w) = \mathbb{K}(\lambda, \Theta(w))/c_v(\Theta(w))$. In view of this latter description, the Similarly, the Gibbs energy (1.7.1) shall also be considered rather in terms of the enthalpy as

$$\mathcal{G}_{\text{therm}}(t, q, w) = \mathcal{G}^{\star}_{\text{therm}}(t, q, \hat{c}_v(\theta)). \tag{1.7.4}$$

At last, the system governing the thermodynamic evolution of SMAs is conjured in the following form:

$$\begin{aligned} \partial_\nu \mathcal{G}_{\text{therm}}(t, q, w) &\ni 0 && \text{in } (0, T) \times \Omega, \\ \partial R_{\text{therm}}(\dot{\lambda}) + [\mathcal{G}_{\text{therm}}]'_\lambda(t, q, w) &\ni 0 && \text{in } (0, T) \times \Omega, \\ \dot{w} - \operatorname{div}(\mathcal{K}\nabla w) &= \delta^*_S(\dot{\lambda}) + \alpha|\dot{\lambda}|^q + \Theta(w)\vec{a} \cdot \dot{\lambda} && \text{in } (0, T) \times \Omega, \\ q(0) = q_0, \quad \Theta(w_0) &= \theta_0 && \text{in } \Omega, \\ y(x) &= y_D(x) && \text{on } [0, T] \times \Gamma_D, \\ (\mathcal{K}\nabla w)n + b\Theta(w) &= b\theta_{\text{ext}} && \text{on } [0, T] \times \partial\Omega. \end{aligned} \tag{1.7.5}$$

An appropriate mixed energetic*times*weak solution concept can then be established.

Definition 1.7.1 (cf. [18]). A quadruple (y, ν, λ, w) such that

$$
\begin{aligned}
y &\in B(0,T; W^{1,p}(\Omega;\mathbb{R}^3)),\\
\nu &\in \left(\mathcal{G}^p(\Omega;\mathbb{R}^{3\times 3})\right)^{[0,T]},\\
\lambda &\in W^{1,q}(0,T;L^q(\Omega)),\\
w &\in L^1(0,T;W^{1,1}(\Omega)),
\end{aligned}
$$

and $\nabla y(t) = id \bullet \nu(t)$ for all $t \in [0,T]$ and a.e. in Ω, and $y(t) = y_D$ on $[0,T]\times\Gamma_D$ is called a weak solution of (1.7.5), if it satisfies

(i) the initial conditions $y(0) = id$, $\nu(0) = \nu_0$, $\lambda(0) = \lambda_0$, $\Theta(w_0) = \theta_0$;

(ii) the minimization principle

$$
\mathcal{G}_{\text{therm}}(t, y(t), \nu(t), \lambda(t), w(t)) \le \mathcal{G}_{\text{therm}}(t, y^\star, \nu^\star, \lambda(t), w(t)),
$$

at every time $t \in [0,T]$ and every $(y^\star, \nu^\star) \in; W^{1,p}(\Omega;\mathbb{R}^3)\times\mathcal{G}^p(\Omega;\mathbb{R}^{3\times3})$ such that $\nabla y^\star = id \bullet \nu^\star$ a.e. in Ω;

(iii) the flow rule

$$
\int_0^T \int_\Omega (\Theta(w) - \theta_{\text{tr}})\vec{a}\cdot(v-\dot\lambda) + \frac{\alpha}{q}|v|^q + \delta_S^*(v)
+ 2(\lambda - \mathcal{L}\bullet\nu, v-\dot\lambda)_{H^{-1}}\,\mathrm{d}x\,\mathrm{d}t \le \int_0^T\int_\Omega \frac{\alpha}{q}|\dot\lambda|^q + \delta_S^*(\dot\lambda)\,\mathrm{d}x\,\mathrm{d}t
$$

for all $v \in L^q(0,T;L^q(\Omega;\mathbb{R}^{M+1}))$, where $(\cdot,\cdot)_{H^{-1}}$ stands for the inner product in $H^{-1}(\Omega;\mathbb{R}^{M+1})$;

(iv) the enthalpy equation

$$
\int_0^T\int_\Omega \mathcal{K}\nabla w\cdot\nabla\zeta - w\dot\zeta\,\mathrm{d}x\,\mathrm{d}t + \int_0^T\int_{\partial\Omega} b\Theta(w)\zeta\,\mathrm{d}S\,\mathrm{d}t = \int_\Omega w_0\zeta(0)\,\mathrm{d}x
+ \int_0^T\int_{\partial\Omega} b\theta_{\text{ext}}\,\mathrm{d}S\,\mathrm{d}t + \int_0^T\int_\Omega \left(\delta_S^*(\dot\lambda) + \alpha|\dot\lambda|^p + \Theta(w)\vec{a}\cdot\dot\lambda\right)\zeta\,\mathrm{d}x\,\mathrm{d}t,
$$

for every $\zeta \in C^1([0,T]\times\overline{\Omega})$ such that $\zeta(T) = 0$.

As in the latter section, under additional data restrictions there exists a weak solution to (1.7.5) in the sense of (1.7.1).

Theorem 1.7.1 (cf. [18]). *Under the data assumptions*

$c(|s|^p - 1) \le \varphi(s) \le C(|s|^p + 1)$ *continuous,* $0 < c < C < +\infty$,
$y_D = id$, $\nu_0 \in \mathcal{G}^p(\Omega;\mathbb{R}^{3\times3})$, $\lambda_0 \in L^q(\Omega)$, $q \ge 2$, $\theta_0 \ge 0$, $\hat c_v(\theta_0) = w_0 \in L^1(\Omega)$,
$f \in W^{1,\infty}(0,T;L^{p^{*\prime}}(\Omega;\mathbb{R}^3))$, $\quad g \in W^{1,\infty}(0,T;L^{p^{\#\prime}}(\Gamma_N;\mathbb{R}^3))$,
$c_1(1+\theta)^{\omega_1-1} \le c_v(\theta) \le c_2(1+\theta)^{\omega_2-1}$, *continuous,* $c_1, c_2 > 0$, $q' \le \omega_1 \le \omega_2$,
$\mathcal{K}(\lambda, w)$ *continuous, bounded and elliptic,*
$\theta_{ext} \in L^1(0,T;L^1(\partial\Omega))$, $\theta_{ext} \ge 0$, $\quad b \in L^\infty(0,T;L^\infty(\partial\Omega))$, $b \ge 0$,

there exists a weak solution to (1.7.5) *in the sense of* (1.7.1).

1.8 Thin film theories of static SMA modelling

A regular way to obtain a thin-film description of solids is to limit the material thickness to zero, more precisely, having a specimen occupying, for the sake of simplicity, $\Omega_\varepsilon := \omega \times \left(-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}\right)$, where $\omega \subset \mathbb{R}^2$ is an open bounded domain with Lipschitz boundary, lying in the (e_1, e_2)-plane and admitting the unit normal e_3. The associated variational problem – for lucidity, discussed here in its most basic form – can then be defined as

$$\begin{aligned} &\text{minimize} \quad \bar{\mathcal{J}}_\varepsilon(y) := \int_{\Omega_\varepsilon} \varphi(\nabla y)\,\mathrm{d}x, \\ &\text{subject to} \quad y \in \bar{\mathcal{A}}_\varepsilon, \end{aligned} \tag{1.8.1}$$

where $\bar{\mathcal{A}}_\varepsilon := \left\{w \in W^{1,p}(\Omega_\varepsilon; \mathbb{R}^3) \colon y(x) = x \text{ on } \Gamma_\varepsilon := \partial\omega \times \left(-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}\right)\right\}$, $1 < p < \infty$, that is, we impose Dirichlet boundary condition on the deformation at the "lateral part" of the specimen boundary.

We are then interested in the limit behaviour of an appropriately chosen diagonal sequence of minimizers y^{ε_n}, $\varepsilon_n \to 0_+$ as $n \to \infty$, i.e.,

$$\bar{\mathcal{J}}_{\varepsilon_n}(y^{\varepsilon_n}) \le \inf_{w \in \bar{\mathcal{A}}_{\varepsilon_n}} \bar{\mathcal{J}}_{\varepsilon_n}(w) + \varepsilon_n h(\varepsilon_n), \tag{1.8.2}$$

for some positive function $h \colon \mathbb{R}^+ \to \mathbb{R}^+$ that tends to zero as $\varepsilon \to 0_+$.

To process integrals over parameter-dependent domains, the general strategy is to change the coordinate system through $z \colon \Omega_1 \to \Omega_\varepsilon$ and consider the rescaled energy by a factor of $\frac{1}{\varepsilon}$. This leads to the rescaled version of (1.8.1), namely

$$\begin{aligned} &\text{minimize} \quad \mathcal{J}_\varepsilon(y) := \int_{\Omega_1} \varphi\left(\nabla_p y \middle| \frac{1}{\varepsilon} y_{,3}\right) \mathrm{d}z, \\ &\text{subject to} \quad y \in \mathcal{A}_\varepsilon, \end{aligned} \tag{1.8.3}$$

where $\nabla_p y := y_{,1} \otimes e_1 + y_{,2} \otimes e_2$ denotes the in-plane gradient of the deformation, $(a_1|a_2|a_3) := a_1 \otimes e_1 + a_2 \otimes e_2 + a_3 \otimes e_3$ – that is, in this case the columns of the given matrix – and the rescaled set of admissible deformations is $\mathcal{A}_\varepsilon := \left\{w \in W^{1,p}(\Omega_1; \mathbb{R}^3) \colon y(z) = (z_1, z_2, \varepsilon z_3)^\top \text{ on } \Gamma_1\right\}$. The transformed version of the diagonal minimizing assumption (1.8.2) then in turn reads as

$$\mathcal{J}_{\varepsilon_n}(y^{\varepsilon_n}) \le \inf_{w \in \mathcal{A}_{\varepsilon_n}} \mathcal{J}_{\varepsilon_n}(w) + h(\varepsilon_n). \tag{1.8.4}$$

Let us further define the set of admissible thin film deformations as

$$\bar{\mathcal{A}}_0 = \left\{w \in W^{1,p}(\Omega_1; \mathbb{R}^3) \colon w_{,3} = 0,\, w(z) = (z_1, z_2, 0)^\top \text{ on } \Gamma_1\right\},$$

which is canonically isomorphic to

$$\mathcal{A}_0 = \left\{w \in W^{1,p}(\omega; \mathbb{R}^3) \colon w(z_p) = (z_1, z_2, 0)^\top \text{ on } \partial\omega\right\}.$$

The first results on non-convex-energy thin films was obtained by Le Dret and Raoult [30]. As a limiting energy they arrived at the quasiconvex envelope of the effective energy density $\varphi_{\text{eff}} \colon \mathbb{R}^{3\times 2} \to \mathbb{R}$, given by

$$\varphi_{\text{eff}}(\bar{F}) = \inf_{z \in \mathbb{R}^3} \varphi(\bar{F}|z).$$

Theorem 1.8.1 (see [30]). *Let ε_n be a sequence that tends to zero for $n \to \infty$. Under the growth assumption*

$$c(|s|^p - 1) \le \varphi(s) \le C(|s|^p + 1) \quad \textit{for some } 0 < c \le C, \textit{ and all } s \in \mathbb{R}^{3\times 3}$$

any minimizing sequence $\{y^{\varepsilon_n}\}_{n\in\mathbb{N}} \in \mathcal{A}_{\varepsilon_n}$ satisfying (1.8.4) *is relatively weakly compact in $W^{1,p}(\Omega_1;\mathbb{R}^3)$. Its limit points $\bar{y}_0$ belong to $\bar{\mathcal{A}}_0$ and can be identified with the solutions $y_0 \in \mathcal{A}_0$ of the minimization problem*

$$\begin{aligned} &\textit{minimize} \quad \mathcal{J}_0^{LDR}(y) := \int_\omega Q\varphi_{\mathit{eff}}(\nabla_p y)\, dz_p, \\ &\textit{subject to} \quad y \in \mathcal{A}_0. \end{aligned} \tag{1.8.5}$$

Later, Freddi and Paroni [42] extended the analysis into the realm of (gradient) Young measures in order to reflect on the underlying microstructure as well. They extended the energy functional

$$\mathcal{J}_\varepsilon^{\mathrm{M}}(\mu) = \begin{cases} \mathcal{J}_\varepsilon(y), & \text{if } \mu = \delta_{\nabla u}, \text{ for some } u \in \mathcal{A}_\varepsilon \\ +\infty, & \text{otherwise in } L_w^\infty(\Omega_1; \mathrm{rca}(\mathbb{R}^{3\times 3})). \end{cases} \tag{1.8.6}$$

When a sequence $\varepsilon_n \to 0_+$, $n \to \infty$ and corresponding $\{\mu_n\}$ is chosen in such a way that the respective energies (1.8.6) are finite, equi-coercivity of the energy functionals can be shown in the following subspace of L^p-gradient Young measures

$$\begin{aligned} \mathcal{G}_0^p(\Omega;\mathbb{R}^{3\times 3}) := \big\{&\mu \in \mathcal{G}^p(\Omega;\mathbb{R}^{3\times 3})\colon \text{the underlying deformation} \\ &\text{satisfies the boundary condition } y(x) = (x_1, x_2, 0)^\top \text{ for } x \in \Gamma_1,\ \pi_\#^3\mu = \delta_0\big\}, \end{aligned}$$

where $\pi_\#^3$ is the image measure corresponding to the projection of $\mathbb{R}^{3\times 3}$ onto $\mathbb{R}^3$ through $\pi^3\colon (a_1|a_2|a_3) \mapsto a_3$. Similarly we define $\pi^p\colon (a_1|a_2|a_3) \mapsto (a_1|a_2)$ and its corresponding image measure $\pi_\#^p$.

Further, the existence of a weak-$\star$ limit $\mu_0 \in \mathcal{G}_0^p(\Omega;\mathbb{R}^{3\times 3})$ in $L_w^\infty(\Omega;\mathrm{rca}(\mathbb{R}^{3\times 3})$ of $\{\mu_n\}$ can be shown. Note that it is however not guaranteed that μ is independent of x_3 in the end. Therefore the authors introduced an average-projection mapping $q\colon L_w^\infty(\Omega;\mathrm{rca}(\mathbb{R}^{3\times 3})) \to L_w^\infty(\omega;\mathrm{rca}(\mathbb{R}^{3\times 2}))$ as

$$\big\langle q(\nu)_{z_p}, \psi\big\rangle := \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{\mathbb{R}^{3\times 2}} \psi(\bar{A})\, \mathrm{d}\pi_\#^p \nu_{(z_p,z_3)}(\bar{A})\, \mathrm{d}z_3, \quad \forall z_p \in \omega\ \forall \psi \in C_0^\infty(\mathbb{R}^{3\times 2}),$$

and, exploiting the technique of Anzellotti, Baldo and Percivale [4], through a modified Γ-convergence they proved the following dimension reduction result.

Theorem 1.8.2 (see [42]). *Let the assumptions of Theorem 1.8.1 hold. Then every minimizing sequence $\{y^{\varepsilon_n}\}_{n\in\mathbb{N}} \in \mathcal{A}_{\varepsilon_n}$ satisfying* (1.8.4) *admits a subsequence (not relabelled) such that*

$$q\left(\delta_{\nabla y^{\varepsilon_n}}\right) \stackrel{*}{\rightharpoonup} \nu \quad \textit{in } L_w^\infty(\omega;\mathrm{rca}(\mathbb{R}^{3\times 2}))$$

for some $\nu \in \mathcal{G}_0^p(\omega;\mathbb{R}^{3\times 2})$ – which means that ν is an L^p-gradient Yound measure and its underlying deformation $y \in W^{1,p}(\omega;\mathbb{R}^3)$ satisfies the boundary condition $y(z_p) = (z_1, z_2, 0)^\top$ for $z_p \in \partial\omega$ – that is the solution of the limit minimization problem

$$\begin{aligned} &\textit{minimize} \quad \mathcal{J}_0^{FP}(\mu) := \int_\omega \int_{\mathbb{R}^{3\times 2}} \varphi_0(\bar{F})\, d\mu_{z_p}(\bar{F})\, dz_p, \\ &\textit{subject to} \quad \mu \in \mathcal{G}_0^p(\omega;\mathbb{R}^{3\times 2}). \end{aligned} \tag{1.8.7}$$

The latter analyses were carried out under purely mesoscopic considerations when the equilibrium of the specimen was determined only through the bulk free energy. If an interfacial energy $\kappa\|\nabla^2 y\|^2_{L^2(\Omega_\varepsilon;\mathbb{R}^{3\times3\times3})}$ is present, Bhattacharya and James [23] derived a limiting Cosserat theory where the deformation of the film is described by two vector fields, separately for the mid-plane $y\colon \omega \to \mathbb{R}^3$ and the cross section $b\colon \omega \to \mathbb{R}^3$ (called the Cosserat vector). More precisely, consider the – rescaled – minimization problem

$$\begin{aligned} &\text{minimize} \quad \mathcal{J}_{\varepsilon,\kappa}(y) := \int_{\Omega_1} \varphi\left(\nabla_p y \middle| \frac{1}{\varepsilon} y_{,3}\right) \\ &\qquad\qquad + \kappa\left(|\nabla_p^2 y|^2 + \frac{2}{\varepsilon^2}|\nabla_p y_{,3}|^2 + \frac{1}{\varepsilon^4}|y_{,33}|^2\right) \mathrm{d}z, \\ &\text{subject to} \quad y \in \mathcal{A}_\varepsilon \cap W^{2,2}(\Omega_1;\mathbb{R}^3). \end{aligned} \tag{1.8.8}$$

Theorem 1.8.3 (see [23])**.** *Let ε_n be a sequence that tends to zero for $n \to \infty$. Under the growth assumption*

$$c(|s|^2 - 1) \le \varphi(s) \le C(|s|^6 + 1) \quad \textit{for some } 0 < c \le C, \textit{ and all } s \in \mathbb{R}^{3\times3}$$

the family of minimizers $\{y^{\varepsilon_n}\}_{n\in\mathbb{N}} \subset W^{2,2}(\Omega_1;\mathbb{R}^3)$ admits a subsequence (not relabelled) such that

$$\begin{aligned} \nabla_p^2 y^{\varepsilon_n} &\to \nabla_p^2 y_0 && \textit{in } L^2(\Omega_1;\mathbb{R}^{3\times2\times2}), \\ \frac{1}{\varepsilon_n}\nabla_p y^{\varepsilon_n}_{,3} &\to \nabla_p b_0 && \textit{in } L^2(\Omega_1,\mathbb{R}^{3\times3}), \\ \frac{1}{\varepsilon_n^2} y^{\varepsilon_n}_{,33} &\to 0 && \textit{in } L^2(\Omega_1,\mathbb{R}^3), \end{aligned}$$

where (y_0, b_0) are independent of z_3 and solve the limiting problem

$$\begin{aligned} &\textit{minimize} \quad \mathcal{J}^{BJ}_{0,\kappa}(y,b) := \int_\omega \varphi(\nabla_p y|b) + \kappa\left(|\nabla_p^2 y|^2 + 2|\nabla_p b|^2\right) dz_p, \\ &\textit{subject to} \quad (y,b) \in W^{2,2}(\omega;\mathbb{R}^3) \times W^{1,2}(\omega;\mathbb{R}^3), \\ &\qquad\qquad\quad y(z_p) = (z_1, z_2, 0),\ b(z_p) = 0 \ \textit{on } \partial\omega. \end{aligned} \tag{1.8.9}$$

As far as evolutionary thin film analysis of shape-memory behaviour goes, we not aware of any newer results than our work Benešová, Kružík, Pathó [15] included in Chapter 2.

1.9 Approximation of martensitic minimizers

As seen in the previous sections, existence of martensitic minimizers can be ensured either through quasiconvexification of the energy density, or by ascending to gradient Young measures. On the other hand, it has been shown [50] that quasiconvex functions $\varphi\colon \mathbb{R}^{m\times n} \to \mathbb{R}$ for $m \ge 3$, $n \ge 2$ – which is our case as well – cannot be described “locally”, what makes it extremely hard to find a computationally feasible characterization of quasiconvex functions. Similarly, the set of (gradient) Young measures is also lacking an effective description from a numerical viewpoint. In order to conduct successful computational simulations, useful approximations are at hand.

The quasiconvex envelope of a function admits upper and lower bounds through other means of convexity, namely polyconvexity and rank-one convexity, and the respective envelopes. First let us recall the definitions of the different notions of convexity, for the sake of further purposes, considering the case $m = 3$, $n = 3$.

A function $\varphi\colon \mathbb{R}^{3\times 3} \to \mathbb{R}$ is said to be polyconvex, if there exists a convex $g\colon \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3} \times \mathbb{R} \to \mathbb{R}$ such that $\varphi(A) = g(A, \operatorname{cof} A, \det A)$ for all $A \in \mathbb{R}^{3\times 3}$, where $\operatorname{cof} A = (\det A)A^{-\top}$ stands for the cofactor of A (for a generalization we refer to [5]). Further, f is said to be rank-one convex, if $f(\lambda A + (1-\lambda)B) \leq \lambda f(A) + (1-\lambda)f(B)$, whenever $0 \leq \lambda \leq 1$ and $\operatorname{rank}(A - B) \leq 1$.

It holds that

$$\varphi^{**} \leq P\varphi \leq Q\varphi \leq R\varphi \leq \varphi, \tag{1.9.1}$$

where

$$\begin{aligned} \varphi^{**} &= \sup\{\psi \leq \varphi\colon \psi \text{ convex}\},\\ P\varphi &= \sup\{\psi \leq \varphi\colon \psi \text{ polyconvex}\},\\ R\varphi &= \sup\{\psi \leq \varphi\colon \psi \text{ rank-one convex}\} \end{aligned}$$

are the respective envelopes of φ (for $Q\varphi$ we point back to (1.4.2) and (1.4.3)), as convex finite-valued functions are polyconvex, which are quasiconvex, and in turn quasiconvexity implies rank-one convexity – the reverse implications, on the other hand, are generally invalid, see [25], [82], although an open case still remains, namely whether rank-one convex functions on $\mathbb{R}^{2\times 2}$ are quasiconvex, for special φ some counterexamples are already at hand, e.g., [3] or [79].

There are very few known functions with an analytic expression for their quasiconvex envelope, see e.g. [27], their approximation therefore utilizes the lower polyconvex bound, see [5], [29], [10], and [11], or the upper rank-one convex bound in (1.9.1), for the latter one, the so-called sequential laminates, we refer to [48], [56], [52], [9], and [13]. Let us remind this sequential-laminate result due to Kohn and Strang [48]. Let $R_0\varphi := \varphi$, and for $k = 1, 2, \ldots$ iteratively define

$$\begin{aligned} R_k\varphi(A) := \inf \{&\xi R_{k-1}\varphi(A_0) + (1-\xi)R_{k-1}\varphi(A_1)\colon \\ &A = \xi A_0 + (1-\xi)A_1,\ \operatorname{rank}(A_0 - A_1) = 1\}. \end{aligned} \tag{1.9.2}$$

Then $R\varphi(A) = \lim_{k\to\infty} R_k\varphi(A)$. $R_k\varphi$ is called the k-th order laminate. Note that laminates are not just allowed but observable shape-memory-alloy microstructures in real-life applications [1].

In Chapter 3 our work is exposed where we conduct computational tests on SMA thin films through laminates (1.9.2).

1.10 Weak lower semicontinuity of multiple integrals

Lastly, Chapter 5 introduces our new results [49] concerning on weak lower semicontinuity of multiple integrals along $\mathcal{A}$-free and asymptotically $\mathcal{A}$-free sequences (see the cases 1 and 2 below), $\mathcal{A}$ being a constant-rank first-order differential operator. More precisely, we give necessary and sufficient conditions for

$$\liminf_{k\to\infty} \int_\Omega h(x, u_k(x))\,\mathrm{d}x \geq \int_\Omega h(x, u(x))\,\mathrm{d}x, \tag{1.10.1}$$

where $|h(x,s)| \leq c(1+|s|^p)$, $1 < p < \infty$, is continuous, and possesses a recession function – though possible negative and non-coercive; $u_k \rightharpoonup u$ in $L^p(\Omega;\mathbb{R}^m)$ and

1. $\mathcal{A}u_k = 0$, or
2. $\mathcal{A}u_k \to 0$ in $W^{-1,p}(\Omega;\mathbb{R}^m)$.

It was first in the gradient case, i.e. when $\mathcal{A} = \mathrm{curl}$, that Meyers [57] observed that besides Morrey's quasiconvexity [62] the behaviour of h at the boundary of Ω plays an important role as well when the p-growth assumption is weakened, see also [51]. When possessing a recession function, Ball and Marsden [8] found that the so-called quasiconvexity at the boundary of h is the additional key property to ensure weak lower semicontinuity of the respective integral.

For a more general operator $\mathcal{A}$, but h non-negative, Fonseca's and Müller's [41] $\mathcal{A}$-quasiconvexity is enough to prove (1.10.1) for both 1 and 2. We [49] shed light on the difficulties that possible concentrations at the boundary can cause under weaker growth assumptions on h, and that 1 and 2 cease to be interchangeable, in general.

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Chapter 2

Mathematical modelling of SMA thin films

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ORIGINAL ARTICLE

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A mesoscopic thermomechanically coupled model for thin-film shape-memory alloys by dimension reduction and scale transition

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Abstract We design a new mesoscopic thin-film model for shape-memory materials which takes into account thermomechanical effects. Starting from a microscopic thermodynamical bulk model, we guide the reader through a suitable dimension reduction procedure followed by a scale transition valid for specimen large in area up to a limiting model which describes microstructure by means of parametrized measures. All our models obey the second law of thermodynamics and possess suitable weak solutions. This is shown for the resulting thin-film models by making the procedure described above mathematically rigorous. The main emphasis is, thus, put on modeling and mathematical treatment of joint interactions of mechanical and thermal effects accompanying phase transitions and on reduction in specimen dimensions and transition of material scales.

Keywords Dimension reduction problems · Shape-memory alloys · Parameterized measures · Thermomechanics

Mathematics Subject Classification (2000) 9S05 · 74N15 · 74N20 · 80A17

1 Introduction

Shape-memory alloys (SMAs) belong to the group of so-called *smart* materials owing to their outstanding response to thermal and/or mechanical loads. In particular, they exhibit the *shape-memory effect* related to recovery from deformation by heat supply. The remarkable behavior of SMAs is due to a diffusionless solid-to-solid phase transition (*martensitic transformation*) characterized by a change in the crystal lattice; in particular, the specimen can transit from a phase of higher symmetry of the crystal lattice, called *austenite*, to a phase with a less symmetric lattice, referred to as *martensite*. Martensite exists in many symmetry-related variants. Hence, the aforementioned phase transition is often accompanied by fast spatial oscillations of the deformation gradient in martensite, the so-called *microstructure*. A SMA specimen can, then, by restructuring

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this microstructure (sometimes referred to as *reorientation*) compensate mechanical loads, which is a key ingredient for its thermomechanical response.

Due to their particular multiscale character, when changes of the crystal lattice lead to extra-ordinary response on macroscale, SMAs have been in the scope of research of physicists, mathematicians and engineers for the last decades, cf. the monographs [10,18,27,37,40] for example. In particular, developing reliable models on various time and length scales as well as surpassing scales is still a big challenge to these communities [39].

Models of the behavior of SMAs then serve for experiment interpretation or when tailoring SMA samples to a specific application area like to surgical tools or stents (for which SMAs are already widely used nowadays [21]); cf. [46] also for other applications. Thus, a large number of models has been developed for specific scales and/or loading regimes, see, e.g., [44] for a survey.

Within this contribution, we consider only continuum-mechanics-based models operating on the single-crystalline level. Following [44], such models can be divided into *microscopic* and *mesoscopic* ones; the crucial difference is that microscopic models operate on the scale of several μm's and record fully the oscillations of the deformation gradient while mesoscopic models record only asymptotics of fine oscillations, e.g., in terms of Young measures generated by gradients (cf. [29]) and are suited for laboratory-sized specimen. Even though, as mentioned, the modeling effort has been large in the past decades, a model for single-crystalline SMAs on the mesoscopic scale that would reflect the thermomechanically coupled nature of SMAs has been proposed only very recently [8].

The main goal of this contribution is to *adapt* the aforementioned model [8] to the *special geometry of thin films*. Indeed, this adaptation is of importance since thin-film specimens are widely used for their microactuator behavior in micro-electro-mechanical (MEMS) devices as they are able to form, under certain circumstances, tents and tunnels [11,19,36]. They profit from the fact that the sizes of these components can be reduced significantly without affecting their functionality that, as explained above, stems merely from crystallographic changes; hence, actuators from SMAs possess a significant power–weight ratio [38].

Dimension reduction, i.e., the rigorous limit procedure when one dimension of the specimen becomes negligible, forms an important tool for obtaining models for the thin-film geometry. In the context of SMAs, this 3D–2D dimension reduction has been performed in the static case; see [11] for the static analysis on the micro- or [31] on the macro-scale (the transition from the first to the latter was shown by Shu [38][48]), or on a purely mesoscopic level [3,15,25,32]; similar procedures are used also in the context of multimaterials [9]. A general framework in rate-independent evolutionary system has been analysed in [34]. Nevertheless, a dimension reduction in the evolutionary mesoscopic model capturing thermomechanical coupling is, to our best knowledge, still missing in the literature.

Thus, we fill this gap by rigorously deriving a thin-film model in the thermomechanically coupled setting. To reach this goal, we propose (see Sect. 2) a two-step procedure: starting from the microscopic thermodynamically consistent hyperelastic bulk model [8], we perform the dimension reduction and then we upscale to a mesoscopic model.

This paper is structured as follows. First, in Sect. 2, we review bulk and thin-film microscopic models which are a starting point of our consideration and which furnish us with ingredients needed for the limiting mesoscopic one. Then, in Sect. 3, we review the existence of a suitably defined weak solution to the microscopic model and, in Sect. 4, we pass to a thin-film limiting model as the material thickness goes to zero. Finally, Sect. 5 is devoted to the existence of a weak solution to a mesoscopic model stemming from the microscopic one by omitting surface energy terms.

2 Considered models and captured effects

In this section, let us shortly introduce the models considered in this contribution and highlight the main effects they capture. As mentioned, the goal of this contribution is to develop a mesoscopic, thermomechanically coupled model in the thin-film geometry. In order to achieve this, we perform the following two-step limiting procedure

$$\text{Microscopic bulk model} \rightarrow \text{Microscopic thin-film model} \rightarrow \text{Mesoscopic thin-film model,}$$

i.e., we consider a thermomechanically coupled model for bulk SMAs that fully resolves the microstructure and let one dimension of the specimen vanish in the first step. Thus, we obtain a thin-film model that is again thermomechanically coupled and fully resolves the microstructure (*microscopic thin-film model*). In this model, we perform then the upscaling for thin films large in area to obtain the mesoscopic thin-film model. This sequence of reasoning is kept throughout the article.

One might also consider following another path, namely, to pass first to a mesoscopic bulk model and then perform the dimension reduction. However, as argued in [17], in the case of ferromagnetics, mesoscopic models form a good approximation of the microscopic ones when the size of the specimen becomes in *all* directions much larger than the size of the associated microstructure. On the other hand, during the dimension reduction procedure, the size of the specimen in a certain direction converges to zero becoming thus less and less dominant over the microstructure size.

Therefore, we consider the former path—dimension reduction followed by scale transition—physically more appropriate. One might still want to consider, e.g., a joint limiting procedure as in [15]. There is no indication the two different approaches should yield the same result.

Our analysis is restricted to single-crystal materials as in [11]. Although shape-memory thin films are typically polycrystals, single-crystal films have as well been produced [20,50]. Nevertheless, we believe that our model can be extended to polycrystals; however, various scaling limits depending on the aspect ratio between film thickness and grain size [48] would make the analysis much more complicated; therefore, we refrain from this scenario here.

2.1 Microscopic bulk model

The starting point of our analysis shall be a microscopic bulk model, analogous to [8], defined in the framework of generalized standard materials, cf. [28]. Take $\Omega_\varepsilon \subset \mathbb{R}^3$ (the reference configuration of the body), $\varepsilon > 0$, such that

$$\Omega_\varepsilon := \omega \times (0, \varepsilon) \quad \text{for some} \quad \omega \subset \mathbb{R}^2, \tag{1}$$

as usual in dimension reduction problems; here ω, the plane of the film is a bounded Lipschitz domain in the (x_1, x_2) plane with disjoint boundary segments $\gamma_{\rm D} \cup \gamma_{\rm N} \cup N = \partial\omega$, where $\gamma_{\rm D}$ is the part of the boundary where Dirichlet boundary condition is prescribed, on $\gamma_{\rm N}$, we demand a Neumann boundary conditions and N is a null set; moreover, ε is the thickness measure of the body. Furthermore, time $t \in [0, T]$ shall be considered on a finite time horizon $0 < T < +\infty$, and we denote $Q_\varepsilon := [0, T] \times \Omega_\varepsilon$ the space-time cylinder, its boundary $\Sigma^\varepsilon := [0, T] \times \partial\Omega_\varepsilon$, while $\Sigma^\varepsilon_{\rm N} := [0, T] \times \Gamma^\varepsilon_{\rm N}$ for $\Gamma^\varepsilon_{\rm N} := \gamma_{\rm N} \times (0, \varepsilon)$; $\Sigma^\varepsilon_{\rm D}$ and $\Gamma^\varepsilon_{\rm D}$ analogously.

In what follows, $y(t)\colon \Omega_\varepsilon \to \mathbb{R}^3$ will denote the deformation of Ω_ε at each time instant $t \in [0, T]$. The set of state variables further includes the *temperature* $\theta : Q_\varepsilon \to \mathbb{R}$ and an internal variable, namely, a vectorial *phase field* $\lambda : Q_\varepsilon \to \mathbb{R}^{M+1}$ that, up to small mismatch, corresponds to the vector of volume fractions of the variants of martensite and/or the austenite phase. Indeed, when assuming that the considered material can exist in $M \in \mathbb{N}$ variants of martensite, together with the austenite, we have possible $M + 1$ states of the specimen. Hence, we may introduce $\mathscr{L} : \mathbb{R}^{3\times 3} \to \mathbb{R}^{M+1}$ a continuous, frame-indifferent (i.e., $\mathscr{L}(F) = \mathscr{L}(RF)$ for every $R \in {\rm SO}(3)$ and every $F \in \mathbb{R}^{3\times 3}$), bounded mapping such that

$$\mathscr{L}(\nabla y)_i = \begin{cases} \text{volume fraction of the } i\text{-th variant of martensite} & \text{if } i \le M, \\ \text{volume fraction of austenite} & \text{if } i = M + 1; \end{cases}$$

e.g., $\mathscr{L}(\cdot)_i$ can be chosen such that it equals one near the respective well and vanishes far from it [30]. We then assume that $\lambda \sim \mathscr{L}(\nabla y)$, the size of the mismatch is controlled by the penalty term in (2). Moreover, we follow the modeling assumption that the evolution of the internal variable leads to energy dissipation (so, indirectly, change of the ratio of the martensitic variants and/or austenite phase leads to dissipation).

Within the framework of generalized standard solids, we have to constitutively define two potentials: the Gibbs free energy $\mathscr{G}^\varepsilon_\eta$ and a dissipation potential $\mathscr{R}^\varepsilon_\eta$ (the two parameters denote the dependence on both the bulk thickness ε and the parameter η governing microscopic effects). Here, we confine ourselves to the following forms of the two potentials:

$$\mathscr{G}^\varepsilon_\eta(t, y, \lambda, \theta) = \underbrace{\int_{\Omega_\varepsilon} H(\nabla y, \lambda, \theta)\,{\rm d}x}_{\text{Helmholtz free energy}} - \underbrace{\int_{\Omega_\varepsilon} f(t)\cdot y\,{\rm d}x - \int_{\Gamma^\varepsilon_{\rm N}} g(t)\cdot y\,{\rm d}S}_{\text{external loading}}$$
$$+\eta\underbrace{\left(\|\nabla^2 y\|^2_{L^2(\Omega_\varepsilon;\mathbb{R}^{3\times3\times3})} + \|\nabla\lambda\|^2_{L^2(\Omega_\varepsilon;\mathbb{R}^{(M+1)\times 3})}\right)}_{\text{interfacial energy}} + \kappa\underbrace{\|\lambda - \mathscr{L}(\nabla y)\|^2_{W^{-1,2}(\Omega_\varepsilon;\mathbb{R}^{M+1})}}_{\text{penalty term}} \tag{2}$$

following [22,42], we propose the following partially linearized ansatz

$$H(F,\lambda,\theta) := W(F) + Z(\theta) + (\theta-\theta_{\rm tr})\mathfrak{a}\cdot\lambda, \quad \forall F \in \mathbb{R}^{3\times3},\ \lambda \in \mathbb{R}^{M+1},\ \theta > 0, \tag{3}$$

where $\theta_{\rm tr} > 0$ is the temperature at which austenite and martensite are energetically equal, W is the purely mechanic part of the Helmholtz free energy, Z purely thermal part and $\mathfrak{a} := (0, 0, \ldots, 0, -s_{\rm tr})^\top$ with $s_{\rm tr}$ being a specific transformation entropy, which corresponds, roughly, to the Clausius–Clapeyron constant multiplied by the transformation strain, cf. [4,30]. Also, the transformation entropy is proportional to the latent heat. Let us note that the thermomechanical coupling term is the leading order in the *chemical energy* [49].

The range of temperatures where such an approximation holds has to be determined for the particular SMAs individually as it is, as mentioned in [49], essentially given by the ratio of the difference in heat capacities between austenite and martensite and the transformation entropy—the latter being commonly much larger.

When choosing W of a multi-well character with the individual wells manifesting the variants of martensite and the austenitic phase, this choice allows the model to predict the formation of microstructure, or in other words, oscillations of the deformation gradient. Now, as the interfacial energy in (2) (the form is chosen following, e.g., [10,37]) has a compactifying effect, the size of the microstructure is controlled by $\sqrt{\eta}$.

To see how does this thermomechanical coupling induces the shape-memory effect, let us begin at high temperature $\theta > \theta_{\rm tr}$. This means that $[(\theta-\theta_{\rm tr})\mathfrak{a}]_{M+1} < 0$, namely, to achieve the smallest Gibbs energy, the material will prefer to reside in the austenite phase. At the transformation temperature $\theta = \theta_{\rm tr}$, as W is presumed to have equally deep wells, there is no energetic distinction between the different phases. And analogously, for low temperatures, $\theta < \theta_{\rm tr}$, the austenite yields a positive contribution to the overall energy through the coupling term, therefore the zero-coupling-energy contributor martensitic phases, recall that $\mathfrak{a} := (0, 0, \ldots, 0, -s_{\rm tr})^\top$, will be given priority in the lattice.

We remark that the interfacial energy term for the volume fraction $\|\nabla\lambda\|^2_{L^2(\Omega_\varepsilon;\mathbb{R}^{(M+1)\times3})}$ is fairly standard in modeling of SMA, see for example [26, Sect. 13.6] or [33] even though other terms allowing for sharp interfaces between variants can be found in an isothermal setting, e.g., in [4,5].

Note that the $W^{-1,2}$ penalization term relaxes the pointwise constraint $\lambda = \mathscr{L}(\nabla y)$, the Lagrange multiplier $\kappa > 0$ considered constant all through, making the mathematical analysis feasible (e.g., an L^2-penalty would require in the weak formulation of the flow rule an L^2-estimate for $\nabla\dot\lambda$, what we do not have at hand).

The dissipation potential is chosen in the form

$$\mathscr{R}^\varepsilon_\eta(\dot y,\dot\lambda) = \int_{\Omega_\varepsilon} \eta|\nabla\dot y| + \frac{\alpha}{q}|\dot\lambda|^q + \delta^*_S(\dot\lambda)\,\mathrm{d}x, \tag{4}$$

with real constants $\alpha > 0$ and $q \geq 2$, the dot standing for $\dot h := \frac{\partial h}{\partial t}$. The last term $\delta^*_S(\dot\lambda)$, the Legendre–Fenchel conjugate of the indicator function of a bounded convex neighborhood S of the origin $0 \in \mathbb{R}^{M+1}$, is considered 1-homogeneous (to capture dissipation due to rate-independent processes—considered dominant) and non-smooth at $\delta^*_S(0)$ (to assure that the change of the phase variable—and, in particular, also the martensite/austenite transition—is an activated process). The term $\frac{\alpha}{q}|\dot\lambda|^q$ corresponds to dissipation due to rate-dependent processes and, in fact, is included mostly for mathematical convenience although models featuring rate dependent dissipation were, at least in the pollyerstatline care, derined recently[13] . Indeed, heat conduction is the dominant cause of rate-dependent effects when the loading frequency is small enough so that we can neglect inertia; cf. Remark 1. So, we consider α sufficiently small so that the rate-dependent term only yields integrability of λ that is needed but does not dominantly contribute to the overall evolution. Finally, the term $\eta|\nabla\dot y|$ models pinning effects, cf. [1], which will vanish on the mesoscopic scale. The chosen, rate-independent, form of the dissipation potential is a modeling issue which is analytically convenient in our situation.

The evolution of the state variables is then standardly [28], in quasistatic approximation, governed by the following inclusions accompanied with the balance of the entropy s:

$$\partial_{\dot y}\mathscr{R}^\varepsilon_\eta(\dot y,\dot\lambda) + \partial_y\mathscr{G}^\varepsilon_\eta(t,y,\lambda,\theta) \ni 0, \tag{5a}$$

$$\partial_{\dot\lambda}\mathscr{R}^\varepsilon_\eta(\dot y,\dot\lambda) + \partial_\lambda\mathscr{G}^\varepsilon_\eta(t,y,\lambda,\theta) \ni 0, \tag{5b}$$

$$\theta\dot s + \operatorname{div} j = \partial\left(\frac{\alpha}{q}|\dot\lambda|^q + \delta^*_S(\dot\lambda)\right)\dot\lambda + \eta|\nabla\dot y|. \tag{5c}$$

In the last equation, j stands for the heat flux and shall be assumed to be governed by the Fourier law, i.e., $j = -\mathbb{K}(\lambda,\theta)\nabla\theta$ with $\mathbb{K}$ being the heat conductivity tensor. Moreover, ∂ is the convex sub-differential which we used in (5a) only formally (since $\mathscr{G}_\eta^\varepsilon(t, y, \lambda, \theta)$ is not convex). We shall give a rigorous weak formulation of the system (5) in Sect. 3—here, for highlighting ideas, we believe the formal system is sufficient.

Remark 1 (*Quasistatic approximation*) The quasistatic approximation considered here is motivated by speed of propagation of the austenite/martensite interface in CuAlNi measured in [47]. In thermal gradient, the speed may be as slow as $10^{-3}\,\mathrm{ms}^{-1}$ which is significantly less than the characteristic speed of wave propagation being around the order $10^3\,\mathrm{ms}^{-1}$. Since the interface propagation is connected to temperature changes, and thus to heat conduction, we include it in our model. On the other hand, we assume that the loading frequency of the specimen is sufficiently low so that inertial effects may be neglected.

Remark 2 (*Boundary conditions*) The system (5), of course, needs to be furnished with appropriate boundary conditions. As it turns out, this is rather nontrivial due to the fact that we included the second gradients in the Gibbs free energy through its interfacial part. Due to this fact, we have to work in the context of so-called *non-simple* continua where boundary conditions have to be prescribed with special care (see e.g., [43]). We shall, thus, assume that the boundary conditions for (5a) in the strong formulation are such that they "vanish" in weak formulation. The entropy equation (5c) is, nonetheless, furnished by Robin-type boundary conditions, cf. Sect. 3.

To summarize, the system (5) records formation of *microstructure of finite width* in martensite as well as its dissipative evolution that is linked to thermal effects, in particular, the shape-memory effect (i.e., recovery from deformation by heat supply) is captured; also, an "inverse" effect is included in the model, namely, the heating/cooling of the specimen during martensitic transformation—since the latent heat in SMAs is typically larger than dissipative effects, the mentioned cooling can indeed be observed [49].

2.2 Microscopic thin-film model

Now when $\varepsilon \to 0_+$ in the potentials (2)–(4), we obtain (after suitable rescaling and a careful limit procedure exposed in Sect. 3) the following "thin-film Gibbs free energy and dissipation potential"

$$\begin{aligned}\mathscr{G}_\eta(t, y, b, \lambda, \theta) = {} & \underbrace{\int_\omega \mathscr{H}(\nabla_p y, b, \lambda, \theta)\,\mathrm{d}z_p}_{\text{in-plane Helmholtz free energy}} \underbrace{- \int_\omega f^0(t)\cdot y\,\mathrm{d}z_p - \int_{\gamma_\mathrm{N}} g^0(t)\cdot y\,\mathrm{d}S_p}_{\text{external force acting in-plane}} \\ & \underbrace{+\eta\Big(\|\nabla_p^2 y\|^2_{L^2(\omega;\mathbb{R}^{3\times2\times2})} + 2\,\|\nabla_p b\|^2_{L^2(\omega;\mathbb{R}^{3\times2})} + \|\nabla_p\lambda\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times2})}\Big)}_{\text{interfacial energy}} \\ & \underbrace{+\kappa\,\big\|\lambda - \mathscr{L}(\nabla_p y|b)\big\|^2_{W^{-1,2}(\omega;\mathbb{R}^{M+1})}}_{\text{penalty term}},\end{aligned} \tag{6a}$$

where $\mathscr{H}(\nabla_p y, b, \lambda, \theta) = W(\nabla_p y|b) + Z(\theta) + (\theta - \theta_{\mathrm{tr}})\mathfrak{a}\cdot\lambda$, and

$$\mathscr{R}_\eta(\dot y, \dot b, \dot\lambda) = \int_\omega \eta|(\nabla_p \dot y|\dot b)| + \frac{\alpha}{q}|\dot\lambda|^q + \delta_S^*(\dot\lambda)\,\mathrm{d}z_p. \tag{6b}$$

So, the potentials (6a) and (6b) are analogous to (2) and (4) but operate only on the two-dimensional domain ω, and, following [11], we obtained a further state variable b that refers to the Cosserat vector and measures the deformation of the cross section of the thin film. All state variables y, b, λ and θ in (6a) will be shown to be independent of the third variable x_3, likewise the external forces: $f^0(t, x_1, x_2) = f(t, x_1, x_2, 0)$, $g^0(t)$ analogously. Consistently, we introduced ∇_p, the in-plane gradient, more precisely,

$$\big(\nabla_p u\big)_{ij} = \partial u_i/\partial x_j \quad \text{for any } u\colon \omega \to \mathbb{R}^d \text{ and } i = 1, \ldots, 3 \text{ and } j = 1, 2; \tag{7}$$

also a point $(x_1, x_2, x_3) \in \Omega_\varepsilon$ consists of an in-plane $x_p = (x_1, x_2)$ and a normal component x_3. Lastly, we introduce the notation $(F|z) \in \mathbb{R}^{3\times3}$ if $F \in \mathbb{R}^{3\times2}$ and $z \in \mathbb{R}^3$ is the last column of the matrix.

With the definition of the two needed potentials at hand, we have the evolution of the thin-film specimen governed by the following system analogous to (5)

$$\partial_{(\dot{y},\dot{b})}\mathscr{R}_\eta(\dot{y},\dot{b},\dot{\lambda}) + \partial_{(y,b)}\mathscr{G}_\eta(t,y,b,\lambda,\theta) \ni 0, \tag{8a}$$

$$\partial_{\dot{\lambda}}\mathscr{R}_\eta(\dot{y},\dot{b},\dot{\lambda}) + \partial_{\lambda}\mathscr{G}_\eta(t,y,b,\lambda,\theta) \ni 0, \tag{8b}$$

$$\theta\dot{s} + \operatorname{div} j = \partial\left(\frac{\alpha}{q}|\dot{\lambda}|^q + \delta_S^*(\dot{\lambda})\right)\dot{\lambda} + \eta\big|(\nabla_p\dot{y}|\dot{b})\big|. \tag{8c}$$

Since the structure of the model is inherited from the bulk model, its main features are analogous to the ones highlighted in the previous subsection.

2.3 Mesoscopic thin-film model

For thin films of large area passing to the limit, $\eta \to 0_+$ is justified by scaling arguments similar to [8,17]; this limit is sometimes referred to as *relaxation*.

In such a case, the interfacial energy vanishes and so the microstructure—or, in other words, oscillations of the deformation gradient—become "infinitely fine"; therefore, we need a suitable mathematical tool to capture this phenomenon. To this end, we employ here the so-called gradient Young measure $\nu \in \mathscr{G}^p_{\Gamma_D}(\Omega;\mathbb{R}^{2\times 3})$ which we shortly introduce in Sect. 5; at this point, it is sufficient to think of them as representatives of the "infinitely fine" microstructure. We use the operator "$\bullet$" to indicate an application of the (gradient) Young measure on its dual, a continuous function with appropriate growth at infinity. For the precise defination see Sect. 5.

In the thin-film geometry, also the Cosserat vector can form fast spatial oscillations additionally to the deformation gradient. This is caused by the fact that a thin film can form an accordion-like structure; if the area of the thin film approaches infinity, also the piling up of the film into the accordion-like structure may become infinitely fine causing again "infinitely fast" oscillations of the Cosserat vector. We capture these by introducing the Young measure $\mu \in \mathscr{Y}^p_{\Gamma_D}(\Omega;\mathbb{R}^3)$.

After passing $\eta \to 0_+$, the Gibbs free energy will read as

$$\mathscr{G}(t,y,\nu,\mu,\lambda,\theta) = \underbrace{\int_\omega W\bullet(\nu,\mu) + Z(\theta) + (\theta-\theta_{\mathrm{tr}})\mathfrak{a}\cdot\lambda(t)\,\mathrm{d}z_p}_{\text{(relaxed) Helmholtz free energy}} + \underbrace{\kappa\|\lambda - \mathscr{L}\bullet(\nu,\mu)\|^2_{W^{-1,2}(\omega;\mathbb{R}^{3\times 3})}}_{\text{mismatch term}}$$
$$\underbrace{-\int_\omega f^0(t)\cdot y\,\mathrm{d}z_p - \int_{\gamma_N} g^0(t)\cdot y\,\mathrm{d}S_p}_{\text{external forces}}, \tag{9}$$

here we denoted $\nabla y = \mathrm{id}\bullet\nu_{z_p}$ for a.a. $z_p \in \omega$ the "average deformation" induced by the microstructure. Notice that the interfacial energy is missing now. Similarly, we scale pinning effects in the dissipation potential to zero and obtain

$$\mathscr{R}(\dot{\lambda}) = \int_\omega \frac{\alpha}{q}|\dot{\lambda}|^q + \delta_S^*(\dot{\lambda})\,\mathrm{d}z_p.$$

Again, the evolution of the state variables is governed by the following set of equations/inclusions:

$$\partial_{(\nu,\mu)}\mathscr{G}(t,y,\nu,\mu,\lambda,\theta) \ni 0, \tag{10a}$$

$$\partial_{\dot{\lambda}}\mathscr{R}(\dot{\lambda}) + \partial_\lambda\mathscr{G}(t,y,\nu,\mu,\lambda,\theta) \ni 0, \tag{10b}$$

$$\theta\dot{s} + \operatorname{div} j = \partial\left(\frac{\alpha}{q}|\dot{\lambda}|^q + \delta_S^*(\dot{\lambda})\right)\dot{\lambda}. \tag{10c}$$

In this system, in particular, (10a) is merely a formal inclusion since the set of gradient Young measures is not convex; therefore, the (convex) subdifferential loses sense here. However, we shall formulate (10a) later, in Sect. 5, via a minimization problem which will, additionally, capture the standard assumption in quasistatic processes that the Gibbs free energy is minimized in every $t \in [0,T]$.

Lastly, let us note that this mesoscopic model does predict several geometric properties of the microstructure, on the other side, the width of the microstructure is not captured anymore. In this approximation, it is so fine that it becomes a characteristic of a single material point—in accord with our intentions with the upscaling. Still, all the important effects stemming from the interplay of formation of microstructure, dissipation and heat conduction in the specimen remain included.

3 Analysis of the microscopic bulk model

Let us now review the weak formulation of (5) and a proof of existence of weak solutions following [7,8,42]. We start with some preparatory paragraphs introducing the necessary notation and the so-called *enthalpy transformation* that will come in handy for the analysis performed later.

To perform the latter, we first transform the entropy equation (5c) into a *heat equation* by employing the standard Gibbs relation $s = -H'_\theta$; thus getting

$$c_{\mathrm{V}}(\theta)\dot{\theta} - \mathrm{div}\,(\mathbb{K}(\lambda,\theta)\nabla\theta) = \frac{\alpha}{q}|\dot{\lambda}|^q + \delta^*_S(\dot{\lambda}) + \eta|\nabla\dot{y}| + \theta\mathfrak{a}\cdot\dot{\lambda}, \tag{11}$$

where $c_{\mathrm{V}}(\theta) = -\theta H''_{\theta\theta}$ is the specific heat capacity. Note that the adiabatic term $+\theta\mathfrak{a}\cdot\dot{\lambda}$ results from the proposed thermomechanical coupling and leads (as already announced) to heating/cooling during phase transition which is actually dominant over the dissipated energy transformed to heat, as observed in experiments [49].

Reformulating this heat Eq. (11) through the enthalpy transformation (cf. [42], for example) by introducing the enthalpy w through

$$w = \hat{c}_{\mathrm{V}}(\theta) = \int_0^\theta c_{\mathrm{V}}(r)\,\mathrm{d}r, \tag{12}$$

one arrives to the relation

$$\dot{w} - \mathrm{div}\,(\mathscr{K}(\lambda,w)\nabla w) = \alpha|\dot{\lambda}|^q + \delta^*_S(\dot{\lambda}) + \eta|\nabla\dot{y}| + \Theta(w)\mathfrak{a}\cdot\dot{\lambda}, \tag{13}$$

where

$$\Theta(w) := \begin{cases} \hat{c}_{\mathrm{V}}^{-1}(w) = \theta, & \text{if } w \geq 0, \\ 0, & \text{otherwise} \end{cases}, \qquad \text{and} \qquad \mathscr{K}(\lambda, w) := \frac{\mathbb{K}(\lambda, \Theta(w))}{c_{\mathrm{V}}(\Theta(w))}.$$

We refer to (13) as the *enthalpy equation*; notice that this will be more convenient for our analysis since the time derivative is not multiplied by the specific heat capacity anymore. Let us stress that in more complicated situations—when we do not have the partially linearized ansatz (3) for the Helmholtz free energy—it requires more care to perform the enthalpy transformation (12), cf. [45].

Let us consider the following Robin boundary condition for (13)

$$\big(\mathscr{K}(\lambda,w)\nabla w\big)\cdot n + \mathfrak{b}\Theta(w) = \mathfrak{b}\theta_{\mathrm{ext}} \qquad \text{on } \Sigma^\varepsilon,$$

for $\mathfrak{b}, \theta_{\mathrm{ext}} \in \mathbb{R}$ a given heat transfer coefficient, θ_{ext} a given external temperature; cf. [8].

As far as additional notation is concerned, we will use $\mathfrak{G}^\varepsilon_\eta$ for the "deformation-related" part of the Gibbs free energy

$$\mathfrak{G}^\varepsilon_\eta(t, y(t), \lambda(t), \Theta(w(t))) := \int_{\Omega_\varepsilon} W(\nabla y(t)) + \eta\left|\nabla^2 y(t)\right|^2 + \frac{\kappa}{2}\left|\nabla\Delta^{-1}(\lambda(t) - \mathscr{L}(\nabla y(t)))\right|^2 \mathrm{d}x$$
$$- \int_{\Omega_\varepsilon} f(t)\cdot y(t)\,\mathrm{d}x - \int_{\Gamma^\varepsilon_{\mathrm{N}}} g(t)\cdot y(t)\,\mathrm{d}S,$$

since this is the only part of the energy that contributes to the semi-stability (14).

Further, where it shall be obvious, we will denote the list of arguments of $\mathscr{G}_\eta^\varepsilon$ and $\mathfrak{G}_\eta^\varepsilon$ at time t simply by t, that is,

$$\mathscr{G}_\eta^\varepsilon(t) \equiv \mathscr{G}_\eta^\varepsilon(t, y(t), \lambda(t), \Theta(w(t))), \qquad \mathfrak{G}_\eta^\varepsilon(t) \equiv \mathfrak{G}_\eta^\varepsilon(t, y(t), \lambda(t), \Theta(w(t)))$$

Lastly,

$$(\!(u, v)\!)_\varepsilon = \int_{\Omega_\varepsilon} \nabla\triangle^{-1}u \cdot \nabla\triangle^{-1}v \,\mathrm{d}x$$

will stand for the inner product in $W^{-1,2}(\Omega_\varepsilon; \mathbb{R}^{M+1}) \simeq \big(W_0^{1,2}(\Omega_\varepsilon; \mathbb{R}^{M+1})\big)^*$, while $\mathrm{Var}_h(u; I \times M)$ shall be the time variation of a map u with respect to a continuous function $h \geq 0$, more precisely

$$\mathrm{Var}_h(u; I \times M) := \sup\left\{ \sum_{i=1}^n \int_M h(u(t_i, x) - u(t_{i-1}, x))\,\mathrm{d}x : \right.$$
$$\left. \text{for all partitions } [t_0, t_n] = I,\ n \in \mathbb{N},\ \text{ such that } t_0 < t_1 < \cdots < t_n \right\};$$

we shall omit the space argument $I \times M$ in case $I \times M = Q_\varepsilon$.

3.1 Weak formulation

To define a suitable weak solution of the system (5), we shall call for the energetic solution concept (see e.g., [35]) further adapted to combinations of rate-independent/rate-dependent processes in [42]. Let us note that, for further convenience, we will explicitly express the dependence of the solutions on the parameters ε and η in their notation.

Definition 1 The triple $(y^{\eta,\varepsilon}, \lambda^{\eta,\varepsilon}, w^{\eta,\varepsilon})$ belonging to

$$\begin{aligned}
y^{\eta,\varepsilon} &\in BV(0, T; W^{1,1}(\Omega_\varepsilon; \mathbb{R}^3)) \cap L^\infty(0, T; W^{2,2}(\Omega_\varepsilon; \mathbb{R}^3)),\\
\lambda^{\eta,\varepsilon} &\in W^{1,q}(0, T; L^q(\Omega_\varepsilon; \mathbb{R}^{M+1})) \cap L^\infty(0, T; W^{1,2}(\Omega_\varepsilon; \mathbb{R}^{(M+1)\times 3})),\\
w^{\eta,\varepsilon} &\in L^1(0, T; W^{1,1}(\Omega_\varepsilon)),
\end{aligned}$$

satisfying the boundary condition $y^{\eta,\varepsilon}(t, x) = 0$ on $\Sigma_{\mathrm{D}}^\varepsilon$ which is called a weak solution of the system (5) if the following holds:

1. SEMI- STABILITY:

$$\mathscr{G}_\eta^\varepsilon(t) \leq \mathscr{G}_\eta^\varepsilon(t, \bar{y}, \lambda^{\eta,\varepsilon}(t), \Theta(w^{\eta,\varepsilon}(t))) + \eta \int_{\Omega_\varepsilon} |\nabla\bar{y} - \nabla y^{\eta,\varepsilon}(t)|\,\mathrm{d}x \tag{14}$$

for all $\bar{y} \in W^{2,2}(\Omega_\varepsilon; \mathbb{R}^3)$ such that $\bar{y}(x) = 0$ on $\Gamma_{\mathrm{D}}^\varepsilon$ and all $t \in [0, T]$.

2. DEFORMATION- RELATED ENERGY EQUALITY:

$$\mathfrak{G}_\eta^\varepsilon(T) - \mathfrak{G}_\eta^\varepsilon(0) + \eta\mathrm{Var}_{|\cdot|}(\nabla y^{\eta,\varepsilon}) = \int_0^T [\mathfrak{G}_\eta^\varepsilon]_t'(t) + 2\kappa(\!(\lambda^{\eta,\varepsilon} - \mathscr{L}(\nabla y^{\eta,\varepsilon}), \dot{\lambda}^{\eta,\varepsilon})\!)_\varepsilon\,\mathrm{d}t \tag{15}$$

3. FLOW RULE:

$$\begin{aligned}
&\int_0^s 2\kappa(\!(\lambda^{\eta,\varepsilon} - \mathscr{L}(\nabla y^{\eta,\varepsilon}), v - \dot{\lambda}^{\eta,\varepsilon})\!)_\varepsilon\,\mathrm{d}t\\
&\quad + \int_0^s \int_{\Omega_\varepsilon} (\Theta(w^{\eta,\varepsilon}) - \theta_{\mathrm{tr}})\mathfrak{a}\cdot(v - \dot{\lambda}^{\eta,\varepsilon}) + 2\eta\nabla\lambda^{\eta,\varepsilon}\cdot\nabla v + \frac{\alpha}{q}|v|^q + \delta_S^*(v)\,\mathrm{d}x\mathrm{d}t\\
&\geq \eta\|\nabla\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega_\varepsilon;\mathbb{R}^{M+1})} - \eta\|\nabla\lambda^{\eta,\varepsilon}(0)\|^2_{L^2(\Omega_\varepsilon;\mathbb{R}^{M+1})} + \int_0^s \int_{\Omega_\varepsilon} \frac{\alpha}{q}|\dot{\lambda}^{\eta,\varepsilon}|^q + \delta_S^*(\dot{\lambda}^{\eta,\varepsilon})\,\mathrm{d}x\mathrm{d}t
\end{aligned} \tag{16}$$

for all test functions $v \in L^q(0, T; L^q(\Omega_\varepsilon; \mathbb{R}^{M+1})) \cap L^\infty(0, T; W^{1,2}(\Omega_\varepsilon; \mathbb{R}^{M+1}))$ and all $s \in [0, T]$.

4. ENTHALPY EQUATION:

$$\int_{Q_\varepsilon} \mathscr{K}(\lambda^{\eta,\varepsilon}, w^{\eta,\varepsilon})\nabla w^{\eta,\varepsilon}\cdot\nabla\zeta - w^{\eta,\varepsilon}\dot{\zeta}\,\mathrm{d}x\mathrm{d}t + \int_{\Sigma^\varepsilon} \mathfrak{b}\Theta(w^{\eta,\varepsilon})\zeta\,\mathrm{d}S\mathrm{d}t$$
$$= \int_{Q_\varepsilon} \left(\delta_S^*(\dot{\lambda}^{\eta,\varepsilon}) + \alpha|\dot{\lambda}^{\eta,\varepsilon}|^q + \Theta(w^{\eta,\varepsilon})\mathfrak{a}\cdot\dot{\lambda}^{\eta,\varepsilon}\right)\zeta\,\mathrm{d}x\mathrm{d}t + \eta\int_{\overline{Q}_\varepsilon}\zeta\mathscr{H}_\varepsilon^\eta(\mathrm{d}x\mathrm{d}t)$$
$$+\int_{\Omega_\varepsilon} w_0^{\eta,\varepsilon}\zeta(0)\,\mathrm{d}x + \int_{\Sigma^\varepsilon}\mathfrak{b}\theta_{\mathrm{ext}}\zeta\,\mathrm{d}S\mathrm{d}t \tag{17}$$

for all $\zeta \in C^1(\overline{Q}_\varepsilon)$ such that $\zeta(T) = 0$; the Radon measure $\mathscr{H}_\varepsilon^\eta \in \mathscr{M}(\overline{Q}_\varepsilon)$, representing the heat production stemming from the term $|\nabla\dot{y}|$ in (4), is defined for every closed set $A = [t,s]\times B$, where $[t,s]\subseteq[0,T]$ and $B\subset\Omega_\varepsilon$ a Borel set, as

$$\mathscr{H}_\varepsilon^\eta(A) := \mathrm{Var}_{|\cdot|}(\nabla y^{\eta,\varepsilon}; [t,s]\times B).$$

5. INITIAL CONDITIONS: $y^{\eta,\varepsilon}(0) = y_0$ for some $y_0 \in W^{2,2}(\Omega_\varepsilon;\mathbb{R}^3)$ and $\lambda^{\eta,\varepsilon}(0) = \lambda_0$ in Ω_ε, $\lambda_0 \in L^q(\Omega_\varepsilon;\mathbb{R}^{M+1})$.

Remark 3 (*Weak formulation of the flow rule* (5b)) The weak formulation (16) is a standard weak formulation of the differential inclusion (5b) together with a by parts integration in the term

$$\int_0^s\int_{\Omega_\varepsilon} 2\eta\nabla\lambda^{\eta,\varepsilon}\cdot(\nabla v - \nabla\dot{\lambda}^{\eta,\varepsilon})\,\mathrm{d}x\mathrm{d}t$$
$$\overset{\text{by parts}}{=} \int_0^s\int_{\Omega_\varepsilon} 2\eta\nabla\lambda^{\eta,\varepsilon}\cdot\nabla v\,\mathrm{d}x\mathrm{d}t - \eta\|\nabla\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega_\varepsilon;\mathbb{R}^{M+1})} + \eta\|\nabla\lambda^{\eta,\varepsilon}(0)\|^2_{L^2(\Omega_\varepsilon;\mathbb{R}^{M+1})}.$$

Further, while standardly one would demand only that it holds for $s = T$, we require that the flow rule holds for all $s\in[0,T]$. Notice that if we did not perform the aforementioned by parts integration, both requirements would be equivalent. Indeed, in such a case, taking a test function such that $v\equiv\dot{\lambda}^{\eta,\varepsilon}$ on $(s,T]$ would yield the flow rule for any $s\in[0,T]$ if it were known for $s = T$.

Here, since we used by parts integration, the required weak formulation is a bit *stronger* which shall be advantageous when performing the dimension reduction in Sect. 4.

Remark 4

(i) Note that the second law of thermodynamics holds, i.e., the entropy production will be non-negative, if we can show that $\theta^{\eta,\varepsilon}\geq 0$ (when the assumed positive semi-definiteness of $\mathbb{K}$ holds).
(ii) Definition 1 is indeed selective, cf. [8].

3.2 Change of variables and rescaling

In order to prepare for the dimension reduction performed later, let us change variables in order to work on the fixed domain $\Omega := \Omega_1 = \omega\times(0,1)$ by introducing new coordinates $z\colon \Omega_\varepsilon\to\Omega$ as

$$z(x) := (z_1, z_2, z_3) = (x_1, x_2, x_3/\varepsilon)\quad \forall x = (x_1,x_2,x_3)\in\Omega_\varepsilon. \tag{18}$$

Subsequently, the scaled functionals (with unchanged notation)

$$\mathscr{G}_\eta^\varepsilon = \frac{1}{\varepsilon}\mathscr{G}_\eta^\varepsilon\circ z^{-1} \quad\text{and}\quad \mathscr{R}_\eta^\varepsilon = \frac{1}{\varepsilon}\mathscr{R}_\eta^\varepsilon\circ z^{-1}, \tag{19}$$

in terms of the new variables read as

$$\mathscr{G}^{\varepsilon}_{\eta}(t) = \int_{\Omega} W\left(\nabla'_{\varepsilon} y^{\eta,\varepsilon}(t)\right) + \kappa\left|\nabla'_{\varepsilon}\triangle^{-1}_{\varepsilon}\big(\lambda^{\eta,\varepsilon}(t) - \mathscr{L}(\nabla'_{\varepsilon} y^{\eta,\varepsilon}(t))\big)\right|^2$$
$$+\eta\left(|\nabla^2_p y^{\eta,\varepsilon}(t)|^2 + \frac{2}{\varepsilon^2}|\nabla_p y^{\eta,\varepsilon}_{,3}(t)|^2 + \frac{1}{\varepsilon^4}|y^{\eta,\varepsilon}_{,33}(t)|^2 + |\nabla_p\lambda^{\eta,\varepsilon}(t)|^2 + \frac{1}{\varepsilon^2}|\lambda^{\eta,\varepsilon}_{,3}(t)|^2\right)$$
$$+(\Theta(w^{\eta,\varepsilon}(t)) - \theta_{\mathrm{tr}})\mathfrak{a}\cdot\lambda^{\eta,\varepsilon}(t) - f(t)\cdot y^{\eta,\varepsilon}(t)\,\mathrm{d}z - \int_{\Gamma_{\mathrm{N}}} g(t)\cdot y^{\eta,\varepsilon}(t)\,\mathrm{d}S \tag{20a}$$

and

$$\mathscr{R}^{\varepsilon}_{\eta}(\dot{y}^{\eta,\varepsilon}(t), \dot{\lambda}^{\eta,\varepsilon}(t)) = \int_{\Omega} \eta\left|\nabla'_{\varepsilon}\dot{y}^{\eta,\varepsilon}(t)\right| + \frac{\alpha}{q}|\dot{\lambda}^{\eta,\varepsilon}(t)|^q + \delta^*_S(\dot{\lambda}^{\eta,\varepsilon})\,\mathrm{d}z. \tag{20b}$$

The scaling factor $1/\varepsilon$ corresponds to the stiffness of the material (in linearized elasticity to the Lamé coefficients of order $1/\varepsilon$).

Above, we denoted by $\nabla'_{\varepsilon} g$ the scaled gradient, namely,

$$\nabla'_{\varepsilon} g = \left(\nabla_p g\left|\frac{1}{\varepsilon} g_{,3}\right.\right)$$

with the 3×2 planar component $(\nabla_p g)_{ij}$ of the gradient, cf. (7), and $(g_{,3})_k := \partial g_k/\partial x_3$ for $k = 1, 2, 3$.

The scaled inverse Laplace operator $\triangle^{-1}_{\varepsilon}\colon L^2(\Omega;\mathbb{R}^{M+1}) \to W^{1,2}_0(\Omega;\mathbb{R}^{M+1})$ stands for the relation $\triangle^{-1}_{\varepsilon} g = h$ whenever

$$\int_{\Omega} \nabla'_{\varepsilon} h(z)\cdot\nabla'_{\varepsilon}\varphi(z) - g(z)\varphi(z)\,\mathrm{d}z = 0 \tag{21}$$

for all $\varphi \in C^{\infty}(\Omega;\mathbb{R}^{M+1})$, i.e., in the classical formulation

$$\frac{\partial^2 h_i}{\partial z_1^2} + \frac{\partial^2 h_i}{\partial z_2^2} + \frac{1}{\varepsilon^2}\frac{\partial^2 h_i}{\partial z_3^2} = g_i \quad \text{in } \Omega, \quad \text{for } i = 1,\dots,M+1,$$
$$h_i = 0 \quad \text{on } \partial\Omega, \quad \text{for } i = 1,\dots,M+1.$$

Also, we will keep the notation $(\!(\cdot,\cdot)\!)_{\varepsilon}$, defined as $(\!(f,g)\!)_{\varepsilon} = \int_{\Omega}\nabla'_{\varepsilon}\triangle^{-1}_{\varepsilon} f\cdot\nabla'_{\varepsilon}\triangle^{-1}_{\varepsilon} g\,\mathrm{d}z$, for the scaled inner product in $W^{-1,2}(\Omega)$.

In the same spirit, the transformed initial conditions shall be denoted as

$$\begin{aligned} y^{\eta,\varepsilon}(0,z) &= y_{0,\varepsilon}(z) := y_0(z_p, \varepsilon z_3),\\ \lambda^{\eta,\varepsilon}(0,z) &= \lambda_{0,\varepsilon}(z) := \lambda_0(z_p, \varepsilon z_3),\\ w^{\eta,\varepsilon}(0,z) &= w_{0,\varepsilon}(z) := w_0(z_p, \varepsilon z_3). \end{aligned} \tag{22}$$

In view of (18)–(20), the transformation of Definition 1 of the weak solution is straightforward.

3.3 Data qualification and existence of weak solutions

Throughout the article, we shall use the following data qualifications:

(D1) *Stored energy density*: $W\colon \mathbb{R}^{3\times 3} \to \mathbb{R}$ is continuous and frame-indifferent, and there exist positive real constants c_1 and c_2 satisfying

$$c_1(-1 + |A|^p) \le W(A) \le c_2(1 + |A|^p)$$

for some $2 \le p < 6$ and all $A \in \mathbb{R}^{3\times 3}$.

(D2) *External forces*:

$$f \in W^{1,\infty}(0,T;L^{p^{*'}}(\Omega_\varepsilon;\mathbb{R}^3)), \qquad g \in W^{1,\infty}(0,T;L^{p^{\sharp'}}(\Gamma_{\mathrm{N}}^{\varepsilon};\mathbb{R}^3)),$$

such that $f \circ z^{-1}$ and $g \circ z^{-1}$ (denoted again by f and g) are independent of the thickness ε.

(D3) *Phase distribution function*: $\mathscr{L} : \mathbb{R}^{3\times3} \to \mathbb{R}$ is continuous and bounded.

(D4) *Specific heat capacity*:$c_{\mathrm{v}} : \mathbb{R} \to \mathbb{R}$ is continuous and satisfies the growth

$$c_1(1+\theta)^{\varsigma_1 - 1} \le c_{\mathrm{v}}(\theta) \le c_2(1+\theta)^{\varsigma_2-1}$$

for some real positive constants c_1, c_2 and $q' \le \varsigma_1 \le \varsigma_2$. This assumption will be employed to prove the strong convergence (41) for the temperature.

(D5) *Heat conductivity tensor*: $\mathscr{K} : \mathbb{R}\times\mathbb{R} \to \mathbb{R}^{3\times3}$ is continuous and there exist real positive constants ξ and Ξ such that

$$\mathscr{K}(\lambda, w) \le \Xi, \qquad \chi^\top \mathscr{K}(\lambda, w)\chi \ge \xi|\chi|^2$$

hold for all $\lambda, w \in \mathbb{R}$ and all $\chi \in \mathbb{R}^3$.

(D6) *Initial and boundary data*:

$$\begin{aligned} &\mathfrak{b} \in L^\infty(\Sigma^\varepsilon),\ \mathfrak{b} \ge 0 \quad &&\text{and} \quad &&\theta_{\mathrm{ext}} \in L^1(\Sigma^\varepsilon),\ \theta_{\mathrm{ext}} \ge 0,\\ &y_0 \in W^{2,2}(\Omega_\varepsilon;\mathbb{R}^3), &&\text{and} &&w_0 \in L^1(\Omega_\varepsilon) \text{ with } \theta_0 \ge 0, \end{aligned}$$

and

$$\lambda_0 \in L^q(\Omega_\varepsilon;\mathbb{R}^{M+1}) \quad \text{is independent of } x_3.$$

Remark 5 Note that (D1) excludes the constraint on the Helmholtz free energy that $W(F) \to \infty$ whenever $\det(F) \to 0$, or, in the thin-film setting, whenever the normal of the thin film approaches zero. The results of [2] would allow us to consider such a constraint in the static case when the Cosserat vector is minimized out. Here, however, the interplay between the Cosserat vector and the film normal makes the situation considerably more difficult, and results of [2] are not applicable. Let us also point to [6] for further results on Young measure relaxation considering the non-interpenetration constraint.

To ease notation, we shall from now on use C as a *generic constant* possibly depending on the given data but *never on* ε, η.

Proposition 1 (Existence of a bulk weak solution) *Let (D1)–(D6) hold. Then, for every $\varepsilon > 0, \eta > 0$ fixed, there exists a weak solution of* (5) *in the spirit of Definition* 1 *such that the following a-priori estimates hold:*

$$\|y^{\eta,\varepsilon}(t)\|_{BV(0,T;W^{1,1}(\Omega;\mathbb{R}^3))} \le C\eta^{-1}, \tag{23a}$$

$$\sup_{t\in[0,T]} \|\nabla'_\varepsilon y^{\eta,\varepsilon}(t)\|_{L^p(\Omega;\mathbb{R}^{3\times3})} \le C, \tag{23b}$$

$$\sup_{t\in[0,T]} \left\| \frac{1}{\varepsilon^2} y^{\eta,\varepsilon}_{,33}(t) \right\|_{L^2(\Omega;\mathbb{R}^{3\times3})} \le C\eta^{-1/2}, \tag{23c}$$

$$\sup_{t\in[0,T]} \|\nabla'_\varepsilon y^{\eta,\varepsilon}(t)\|_{W^{1,2}(\Omega;\mathbb{R}^{3\times3})} \le C\eta^{-1/2} \tag{23d}$$

for the deformation,

$$\|\dot\lambda^{\eta,\varepsilon}\|_{L^q(0,T;L^q(\Omega;\mathbb{R}^{M+1}))} \le C, \tag{24a}$$

$$\sup_{t\in[0,T]} \|\nabla'_\varepsilon \lambda^{\eta,\varepsilon}(t)\|_{L^2(\Omega;\mathbb{R}^{(M+1)})} \le C\eta^{-1/2} \tag{24b}$$

for the phase field, and

$$\|w^{\eta,\varepsilon}\|_{L^\infty(0,T;L^1(\Omega))} \le C, \tag{25a}$$

$$\|\nabla'_\varepsilon w^{\eta,\varepsilon}\|_{L^r(0,T;L^r(\Omega;\mathbb{R}^3)} \le C(r) \quad \text{for any } r < \frac{5}{4}, \tag{25b}$$

$$\|\dot w^{\eta,\varepsilon}\|_{\mathscr{M}(0,T;(W^{1,\infty}(\Omega))^*)} \le C \tag{25c}$$

for the enthalpy.

Note that in (25c) $\mathscr{M}$ denotes the set of Radon measures.

Proof The proof follows a rather standard procedure, cf. [7,8] or [42], of showing that the interpolants of a particular discrete approximation converge to the sought bulk solution; therefore, a detailed proof is omitted. Let us, however, sketch its main ingredients.

STEP 1: TIME DISCRETIZATION OF THE WEAK FORMULATION. Define the discrete weak solution of (5) at time level k, $k = 1, \dots, T/\tau$, as a triple $(y_k^\tau, \lambda_k^\tau, w_k^\tau) \in W^{2,2}(\Omega;\mathbb{R}^3) \times L^{2q}(\Omega;\mathbb{R}^{M+1}) \times W^{1,2}(\Omega)$ satisfying

1. TIME- INCREMENTAL MINIMIZATION PROBLEM:

$$\begin{aligned}\text{Minimize}\quad & \mathscr{G}_\eta^\varepsilon(t_k, y, \lambda, \Theta(w_k^\tau)) + \int_\Omega \tau|\lambda|^{2q} + \eta|\nabla'_\varepsilon y - \nabla'_\varepsilon y_{k-1}^\tau| \\ & \qquad + \delta_S^*\left(\frac{\lambda - \lambda_{k-1}^\tau}{\tau}\right) + \frac{\tau\alpha}{q}\left|\frac{\lambda-\lambda_{k-1}^\tau}{\tau}\right|^q \mathrm{d}z \\ \text{subject to}\quad & (y,\lambda) \in W^{2,2}(\Omega;\mathbb{R}^3) \times L^{2q}(\Omega;\mathbb{R}^{M+1}), \\ & y(z) = 0 \quad \text{for } z \in \Gamma_\mathrm{D}. \end{aligned} \tag{26}$$

2. ENTHALPY EQUATION:

$$\begin{aligned}&\int_\Omega \frac{w_k^\tau - w_{k-1}^\tau}{\tau} + \mathscr{K}(\lambda_k^\tau, w_k^\tau)\nabla'_\varepsilon w_k^\tau \cdot \nabla'_\varepsilon \zeta \,\mathrm{d}z + \int_{\partial\Omega} \mathfrak{b}_k^\tau \Theta(w_k^\tau)\zeta - \mathfrak{b}_k^\tau \theta_\mathrm{ext}\zeta \,\mathrm{d}S \\ &= \int_\Omega \delta_S^*\left(\frac{\lambda_k^\tau - \lambda_{k-1}^\tau}{\tau}\right)\zeta + \alpha\left|\frac{\lambda_k^\tau - \lambda_{k-1}^\tau}{\tau}\right|^q\zeta + \left|\frac{\nabla'_\varepsilon y_k^\tau - \nabla'_\varepsilon y_{k-1}^\tau}{\tau}\right|\zeta + \Theta(w_k^\tau)\mathfrak{a}\cdot\left(\frac{\lambda_k^\tau - \lambda_{k-1}^\tau}{\tau}\right)\zeta\,\mathrm{d}z\end{aligned}$$

   for all $\zeta \in W^{1,2}(\Omega)$.

3. INITIAL CONDITIONS:

$$y_0^\tau = y_{0,\varepsilon}, \qquad \lambda_0^\tau = \lambda_{0,\varepsilon}^\tau, \qquad w_0^\tau = w_{0,\varepsilon}^\tau \quad \text{a.e. in } \Omega,$$

   where $\mathfrak{b}_k^\tau, \lambda_{0,\varepsilon}^\tau, w_{0,\varepsilon}^\tau$ are suitable approximations of the original data (D6).

Notice the added regularization term $\int_\Omega \tau|\lambda|^{2q}\,\mathrm{d}z$ allows for a rather standard proof of existence of a discrete weak solution but vanishes as $\tau \to 0$. Details are to be found, e.g., in [7].

STEP 2: A- PRIORI ESTIMATES. Let us outline the proof of the a-priori estimates (23)–(25) merely heuristically, on the continuum level instead of the discrete setting, where a rigorous proof would follow the same ideas but be technically more demanding, cf. [7] again.

First, from the energy equality (15) integrated only to some $s \in [0, T]$ (note that we actually need only the lower inequality—this can be, on the discrete level, got from (26) integrated to any arbitrary $s \in [0, T]$), we get by exploiting the coercivity assumptions (D1) on the left-hand side and the bounds (D2)–(D3) as well as (D6) on the right-hand side

$$\begin{aligned}&\int_\Omega C|\nabla'_\varepsilon y^{\eta,\varepsilon}(s)|^p + \eta\left(\left|\nabla_p^2 y^{\eta,\varepsilon}(s)\right|^2 + 2\left|\frac{1}{\varepsilon}\nabla_p y_{,3}^{\eta,\varepsilon}(s)\right|^2 + \left|\frac{1}{\varepsilon^2}y_{,33}^{\eta,\varepsilon}(s)\right|^2\right)\mathrm{d}z \\ &\quad + \eta\mathrm{Var}_{|\cdot|}(\nabla'_\varepsilon y^{\eta,\varepsilon};\Omega\times[0,s]) \le \int_0^s\int_\Omega \left(\frac{\alpha}{4q}|\dot\lambda^{\eta,\varepsilon}|^q + C|\nabla'_\varepsilon y^{\eta,\varepsilon}|^p\right)\mathrm{d}z\mathrm{d}t + C.\end{aligned} \tag{27}$$

Further, by testing the flow rule (16) (after the change of scale) by $v = 0$ on $[0, s]$ (note that this test essentially executes the standard test of the strong flow rule by $\dot\lambda^{\eta,\varepsilon}$) we get

$$\begin{aligned}&\int_0^s\int_\Omega \delta_S^*(\dot\lambda^{\eta,\varepsilon}) + \frac{\alpha}{q}|\dot\lambda^{\eta,\varepsilon}|^q\,\mathrm{d}z\,\mathrm{d}t + \eta\|\nabla'_\varepsilon\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega_\varepsilon;\mathbb{R}^{(M+1)\times 3})} + \eta\|\nabla_p\lambda_0\|^2_{L^2(\Omega_\varepsilon;\mathbb{R}^{(M+1)\times 2})} \\ &\le -2\kappa\int_0^s (\!(\lambda^{\eta,\varepsilon} - \mathscr{L}(\nabla'_\varepsilon y^{\eta,\varepsilon}), \dot\lambda^{\eta,\varepsilon})\!)_\varepsilon\,\mathrm{d}t + \int_0^s\int_\Omega |\Theta(w^{\eta,\varepsilon}) - \theta_\mathrm{ext}|\cdot|\dot\lambda^{\eta,\varepsilon}|\,\mathrm{d}z\mathrm{d}t,\end{aligned} \tag{28}$$

where we used that $[\lambda_0]_{,3} = 0$ due to (D6). This, after plugging in the by parts integration formula

$$2\int_0^s ((\lambda^{\eta,\varepsilon}, \dot{\lambda}^{\eta,\varepsilon}))_\varepsilon \, dt = \int_\Omega |\nabla'_\varepsilon \Delta_\varepsilon^{-1} \lambda^{\eta,\varepsilon}(s)|^2 - |\nabla'_\varepsilon \Delta_\varepsilon^{-1} \lambda^{\eta,\varepsilon}(0)|^2 \, dz, \tag{29}$$

yields (with the help of Young's inequality and (D6) again) the estimate

$$\int_0^s \int_\Omega \left(\delta_S^*(\dot{\lambda}^{\eta,\varepsilon}) + \frac{\alpha}{q} |\dot{\lambda}^{\eta,\varepsilon}|^q \right) dz dt + \int_\Omega \kappa |\nabla'_\varepsilon \Delta_\varepsilon^{-1} \lambda^{\eta,\varepsilon}(s)|^2 \, dz + \eta |\nabla'_\varepsilon \lambda^{\eta,\varepsilon}(s)|^2 \, dz$$

$$\leq \int_0^s \int_\Omega \frac{\alpha}{4q} |\dot{\lambda}^{\eta,\varepsilon}|^q + C|w| \, dz dt + C. \tag{30}$$

Lastly, testing enthalpy equation (13) by α / lq, with some $l \geq 8$ such that $\alpha \leq lq$, and integrating again over Ω and $[0, s]$ gives (notice that this test can be straightforwardly executed on the discrete level)

$$\frac{\alpha}{lq} \int_0^s \int_\Omega \dot{w}^{\eta,\varepsilon} \, dz dt \leq \int_0^s \int_\Omega \frac{2\alpha}{lq} |\dot{\lambda}^{\eta,\varepsilon}|^q + C|w^{\eta,\varepsilon}| \, dz dt + \frac{\alpha\varepsilon}{lq} \mathrm{Var}_{|\cdot|}(\nabla'_\varepsilon y^{\eta,\varepsilon}; \Omega \times [0, s]) + C. \tag{31}$$

Adding (27), (30) and (31) gives then the bounds (23), (24) and (25a). The estimate (25b) on the scaled gradient of $w^{\eta,\varepsilon}$ follows by fine technique due to [13,14] from the test of the enthalpy equation in (13) by $1 - 1/(1 + w^{\eta,\varepsilon})^\alpha$, while (25c) is a standard dual estimate stemming from the enthalpy equation (17) itself.

Step 3: Convergence $\tau \to 0$: The proof of convergence for $\tau \to 0$ can be performed similarly as in [7,42], or the methods exposed in the proof of Theorem 1 are easily applicable to this case, too. □

4 Dimension reduction in the microscopic thin-film model

Let us now concentrate on the microscopic thin-film model given through the system of inclusion/equations (8). As mentioned above, particularly the inclusion (8a) is rather formal; therefore, we propose its weak formulation in the spirit of semi-energetic solutions, due to [42], similarly to the previous section. Also, again, we transformed the heat equation into a enthalpy equation.

4.1 Weak formulation

To shorten the notation, we shall denote hereinafter $\mathcal{Q} := [0, T] \times \omega$, while the in-plane inner product in the space $W^{-1,2}(\omega; \mathbb{R}^{M+1})$ will be denoted as $((u, v))_p := \int_\omega \nabla_p \Delta_p^{-1} u \cdot \nabla_p \Delta_p^{-1} v \, dz_p$, for all $u, v \in W^{-1,2}(\omega; \mathbb{R}^{M+1})$, whereas $\Delta_p^{-1} \colon L^2(\omega; \mathbb{R}^{M+1}) \to W_0^{1,2}(\omega; \mathbb{R}^{M+1})$ is the in-plane inverse Laplace operator, more precisely, $\Delta_p^{-1} g = h$ whenever

$$\int_\omega \nabla_p h(z_p) \cdot \nabla_p \phi(z_p) - g(z_p)\phi(z_p) \, dz_p = 0$$

for every $\phi \in C^\infty(\omega; \mathbb{R}^{M+1})$, i.e., in the classical formulation

$$\frac{\partial^2 h_i}{\partial z_1^2} + \frac{\partial^2 h_i}{\partial z_2^2} = g_i \quad \text{in } \omega, \quad \text{for } i = 1, \ldots, M+1,$$

$$h_i = 0 \quad \text{on } \partial\omega, \quad \text{for } i = 1, \ldots, M+1.$$

Definition 2 Let us call the quadruple $(y^\eta, b^\eta, \lambda^\eta, w^\eta)$ belonging to

$$y^\eta \in BV(0,T;W^{1,1}(\omega;\mathbb{R}^3)) \cap L^\infty(0,T;W^{2,2}(\omega;\mathbb{R}^3)), \tag{32a}$$
$$b^\eta \in BV(0,T;L^1(\omega;\mathbb{R}^3)) \cap L^\infty(0,T;W^{1,2}(\omega;\mathbb{R}^3)), \tag{32b}$$
$$\lambda^\eta \in W^{1,q}(0,T;L^q(\omega;\mathbb{R}^{M+1})) \cap L^\infty(0,T;W^{1,2}(\omega;\mathbb{R}^{M+1})), \tag{32c}$$
$$w^\eta \in L^1(0,T;W^{1,1}(\omega)), \tag{32d}$$

such that $(y^\eta, b^\eta)(t, z_1, z_2) = 0$ for all $t \in [0,T]$ and a.e. on γ_{D}, a weak solution of the evolutionary thin-film problem (8) if it satisfies

1. Semi- stability:
$$\mathscr{G}_\eta(t) \le \mathscr{G}_\eta(t, \bar{y}, \bar{b}, \lambda^\eta(t), \Theta(w^\eta(t))) + \int_\omega \eta \left|\left(\nabla_p y^\eta(t)|b^\eta(t)\right) - \left(\nabla_p \bar{y}|\bar{b}\right)\right| \mathrm{d}z_p \tag{33}$$
for every $(\bar{y}, \bar{b}) \in W^{2,2}(\omega;\mathbb{R}^3) \times W^{1,2}(\omega;\mathbb{R}^3)$ such that $(\bar{y}, \bar{b}) = 0$ a.e. on γ_{D} (recall the definition (6a) of the Gibbs free energy $\mathscr{G}_\eta(t)$);
2. Deformation- related energy equality:
$$\mathfrak{G}_\eta(T) - \mathfrak{G}_\eta(0) + \eta \mathrm{Var}_{|\cdot|}((\nabla_p y^\eta|b^\eta); \mathscr{Q}) = \int_0^T [\mathfrak{G}_\eta]'_t(t) + 2\kappa (\!(\lambda^\eta - \mathscr{L}(\nabla_p y^\eta(t)|b^\eta(t)), \dot{\lambda}^\eta)\!)_p \,\mathrm{d}t \tag{34}$$
where $\mathfrak{G}_\eta(t)$ is defined as
$$\mathfrak{G}_\eta(t) := \int_\omega W(\nabla_p y^\eta|b^\eta) + \eta\left(|\nabla_p^2 y^\eta|^2 + 2|\nabla_p b^\eta|^2\right) \mathrm{d}z_p + \kappa \left\|\lambda^\eta - \mathscr{L}(\nabla_p y^\eta|b^\eta)\right\|^2_{W^{-1,2}(\omega;\mathbb{R}^{M+1})}$$
$$- \int_\omega f^0 \cdot y^\eta \,\mathrm{d}z_p - \int_{\gamma_{\mathrm{N}}} g^0 \cdot y^\eta \,\mathrm{d}S_p; \tag{35}$$
3. Flow rule:
$$\int_0^s 2\kappa (\!(\lambda^\eta - \mathscr{L}(\nabla_p y^\eta(t)|b^\eta(t)), v - \dot{\lambda}^\eta)\!)_p \,\mathrm{d}t$$
$$+ \int_0^s \int_\omega (\Theta(w^\eta) - \theta_{\mathrm{tr}})\mathfrak{a} \cdot (v - \dot{\lambda}^\eta) + 2\eta \nabla_p \lambda^\eta \cdot \nabla_p v + \frac{\alpha}{q}|v|^q + \delta_S^*(v) \,\mathrm{d}z_p \mathrm{d}t$$
$$\ge \eta \|\nabla_p \lambda^\eta(T)\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})} - \eta \|\nabla_p \lambda^\eta(0)\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})} + \int_0^s \int_\omega \frac{\alpha}{q}|\dot{\lambda}^\eta|^q + \delta_S^*(\dot{\lambda}^\eta) \,\mathrm{d}z_p \mathrm{d}t \tag{36}$$
for all test functions $v \in L^q(0,T;L^q(\omega;\mathbb{R}^{M+1})) \cap L^\infty(0,T;W^{1,2}(\omega;\mathbb{R}^{M+1})$ and every $s \in [0,T]$.
4. Enthalpy equation:
$$\int_{\mathscr{Q}} \mathscr{K}(\lambda^\eta, w^\eta)\nabla_p w^\eta \cdot \nabla_p \zeta - w^\eta \dot{\zeta} \,\mathrm{d}z_p \mathrm{d}t + \int_0^T\!\!\int_{\partial\omega} \mathfrak{b}\Theta(w^\eta)\zeta \,\mathrm{d}S_p \mathrm{d}t = \int_\omega w_0 \zeta(0) \,\mathrm{d}z_p$$
$$+ \int_{\mathscr{Q}} \left(\delta_S^*(\dot{\lambda}^\eta) + \alpha|\dot{\lambda}^\eta|^q + (\Theta(w^\eta) - \theta_{\mathrm{tr}})\mathfrak{a} \cdot \dot{\lambda}^\eta\right)\zeta \,\mathrm{d}z_p \mathrm{d}t + \eta \int_{\overline{\mathscr{Q}}} \zeta \mathscr{H}^\eta(\mathrm{d}z_p \mathrm{d}t) + \int_0^T\!\!\int_{\partial\omega} \mathfrak{b}\theta_{\mathrm{ext}}\zeta \,\mathrm{d}S_p \mathrm{d}t \tag{37}$$
for all $\zeta \in C^1(\overline{\mathscr{Q}})$ such that $\zeta(T) = 0$. Analogously to (37), here again the Radon measure $\mathscr{H}^\eta \in \mathscr{M}(\overline{\mathscr{Q}})$, $\eta > 0$ represents the heat production due to $\eta|(\nabla_p \dot{y}|\dot{b})|$ and is defined for any closed set $A = [t,s] \times B$, where $[t,s] \subseteq [0,T]$ and $B \subset \omega$ a Borel set, as
$$\mathscr{H}^\eta(A) := \mathrm{Var}_{|\cdot|}((\nabla_p y^\eta|b^\eta); [t,s] \times B).$$

5. INITIAL CONDITIONS:

$$\begin{aligned} y^\eta(0, z_p) &= y_{0,0}(z_p) := y_0(z_p, 0), \\ b^\eta(0, z_p) &= b_0(z_p) := (y_0)_{,3}(z_p, 0), \\ \lambda^\eta(0, z_p) &= \lambda_{0,0}(z_p) := \lambda_0(z_p, 0), \end{aligned} \tag{38}$$

4.2 Existence of weak solutions

Theorem 1 *Let (D1)–(D6) hold. Then, there exists a quadruple $(y^\eta, b^\eta, \lambda^\eta, w^\eta)$ belonging to the spaces (32) such that $(y^\eta, b^\eta)(t, z_1, z_2) = 0$ for all $t \in [0, T]$ and a.e. on γ_D and a (not relabeled) subsequence $\varepsilon \to 0_+$ such that the following holds*

$$y^{\eta,\varepsilon}(t) \to y^\eta(t) \qquad \text{in } W^{2,2}(\Omega; \mathbb{R}^3) \text{ for all } t \in [0, T], \tag{39a}$$

$$\frac{1}{\varepsilon} y^{\eta,\varepsilon}_{,3}(t) \to b^\eta(t) \qquad \text{in } W^{1,2}(\Omega; \mathbb{R}^3) \text{ for all } t \in [0, T], \tag{39b}$$

$$\lambda^{\eta,\varepsilon} \to \lambda^\eta \qquad \text{in } W^{1,q}(0, T; L^q(\Omega; \mathbb{R}^{M+1})), \tag{39c}$$

$$\nabla'_\varepsilon \lambda^{\eta,\varepsilon} \to (\nabla_p \lambda^\eta | 0) \qquad \text{in } L^2(\Omega; \mathbb{R}^{(M+1)\times 3}) \text{ for all } t \in [0, T] \tag{39d}$$

$$\nabla_p w^{\eta,\varepsilon} \rightharpoonup \nabla_p w^\eta \qquad \text{in } L^r(0, T; L^r(\Omega)) \text{ for any } 1 \le r < \frac{5}{4} \tag{39e}$$

$$w^{\eta,\varepsilon} \to w^\eta \qquad \text{in } L^s(Q) \text{ for any } 1 \le s < \frac{5}{3}, \tag{39f}$$

with $\{(y^{\eta,\varepsilon}, \lambda^{\eta,\varepsilon}, w^{\eta,\varepsilon})\}_{\varepsilon>0}$ a family of weak solutions of (5) obtained in Proposition 1; $(y^\eta, b^\eta, \lambda^\eta, w^\eta)$ is then a weak solution to (8) in the spirit of Definition 2.

Proof For the sake of transparency, let us divide the proof into separate distinct steps.

STEP 1: SELECTION OF SUBSEQUENCES. The a-priori estimates (23) ensure—by Helly's selection principle—the existence of two vector fields $y^\eta \in BV(0, T; W^{1,1}(\Omega; \mathbb{R}^3))$, $b^\eta \in BV(0, T; L^1(\Omega; \mathbb{R}^3))$ such that

$$y^{\eta,\varepsilon}(t) \rightharpoonup y^\eta(t) \qquad \text{in } W^{2,2}(\Omega; \mathbb{R}^3) \text{ for all } t \in [0, T], \tag{40a}$$

$$\frac{1}{\varepsilon} y^{\eta,\varepsilon}_{,3}(t) \rightharpoonup b^\eta(t) \qquad \text{in } W^{1,2}(\Omega; \mathbb{R}^3) \text{ for all } t \in [0, T]. \tag{40b}$$

Similarly, using standard selection and embedding theorems, estimate (24a) ensures the existence of a limit phase field λ^η such that

$$\lambda^{\eta,\varepsilon} \rightharpoonup \lambda^\eta \quad \text{in } W^{1,q}(0, T; L^q(\Omega; \mathbb{R}^{M+1})). \tag{40c}$$

By exploiting further the estimate (24b) and the continuous embedding of the Sobolev space $W^{1,q}(0, T; L^q(\Omega; \mathbb{R}^{M+1}))$ into $C(0, T; L^q(\Omega; \mathbb{R}^{M+1})$, we get that

$$\nabla_p \lambda^{\eta,\varepsilon}(t) \rightharpoonup \nabla_p \lambda^\eta(t) \qquad \text{in } L^2(\Omega; \mathbb{R}^{(M+1)\times 2}) \text{ for all } t \text{ in } [0, T]. \tag{40d}$$

The situation is more complicated for the third component of $\nabla'_\varepsilon \lambda^{\eta,\varepsilon}$, we shall return to it later in Step 3, where also the strong convergence (39d) will be shown. The strong convergences (39a)–(39b) will be obtained in Step 5.

Lastly, we may extract a (not relabeled) subsequence of $\{w^{\eta,\varepsilon}\}_{\varepsilon>0}$ such that (39e) and (39f) are satisfied; notice that the latter convergence stems from the dual estimate (25c) and the generalized Aubin–Lions lemma, cf. [41, Corollary 7.8 and 7.9] and [42, equation (4.55)]. Moreover, (39f) yields, together with the assumption (D4), the strong convergence

$$\Theta(w^{\eta,\varepsilon}) \to \Theta(w^\eta) \quad \text{in } L^{q'}(Q). \tag{41}$$

In order to see this, we exploit the first inequality in assumption (D4)

$$w^{\eta,\varepsilon} = \int_0^{\theta^{\eta,\varepsilon}} c_{\rm v}(r)\,{\rm d}r \geq c_1 \int_0^{\Theta(w^{\eta,\varepsilon})} (1+r)^{\varsigma_1-1}\,{\rm d}r \geq c_1\left((1+\Theta(w^{\eta,\varepsilon}))^{\varsigma_1}-1\right),$$

where we used that $\theta^{\eta,\varepsilon} \geq 0$, together with the assumption $\varsigma_1 \geq q'$ to get the bound

$$|\Theta(w^{\eta,\varepsilon})| \leq C\left(1+|w^{\eta,\varepsilon}|^{1/q'}\right).$$

Hence, by the continuity of the Nemytskii mapping induced by Θ, one arrives to (41).

STEP 2: INDEPENDENCE OF z_3. It follows from the estimates (23d) and the weak lower semicontinuity of the norm that

$$0 = \liminf_{\varepsilon\to 0_+} c\varepsilon \geq \liminf_{\varepsilon\to 0_+} \|y^{\eta,\varepsilon}_{,3}(t)\|_{W^{1,2}(\Omega;\mathbb{R}^3)} \geq \|y^{\eta}_{,3}(t)\|_{W^{1,2}(\Omega;\mathbb{R}^3)} \geq 0.$$

This means that y^η is independent of z_3 for all $t \in [0,T]$. Analogously, the independence of λ^η and b^η of z_3 follows from the estimate (24b), resp. (23c). For w^η, we get that it is independent of z_3 only for a.a. $t \in [0,T]$ from (25b).

STEP 3: THIN-FILM FLOW RULE. Recall the bulk flow (16) which we rescale and in which we expand the matrix ∇'_ε into its planar and normal components, namely

$$\begin{aligned}&\int_0^s\int_\Omega (\Theta(w^{\eta,\varepsilon})-\theta_{\rm tr})\mathfrak{a}\cdot(v-\dot\lambda^{\eta,\varepsilon}) + \frac{\alpha}{q}|v|^q + \delta^*_S(v)\,{\rm d}z{\rm d}t + \int_0^s 2\kappa\,((\lambda^{\eta,\varepsilon}-\mathscr{L}(\nabla'_\varepsilon y^{\eta,\varepsilon}), v-\dot\lambda^{\eta,\varepsilon}))_\varepsilon\,{\rm d}t\\ &\quad+\int_0^s\int_\Omega 2\eta\nabla_p\lambda^{\eta,\varepsilon}\cdot\nabla_p v + \frac{2\eta}{\varepsilon^2}\lambda^{\eta,\varepsilon}_{,3}\cdot v_{,3}\,{\rm d}z{\rm d}t + \eta\|\nabla_p\lambda_0\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}\\ &\geq \eta\|\nabla_p\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})} + \frac{\eta}{\varepsilon^2}\|\lambda^{\eta,\varepsilon}_{,3}(s)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})} + \int_0^s\int_\Omega \frac{\alpha}{q}|\dot\lambda^{\eta,\varepsilon}|^q + \delta^*_S(\dot\lambda^{\eta,\varepsilon})\,{\rm d}z{\rm d}t\end{aligned}$$

where we used that, due to (D6), λ_0 does not depend on the third component. Let us admit *only test functions independent of* z_3 which simplifies the flow rule to

$$\begin{aligned}&\int_0^s\int_\Omega (\Theta(w^{\eta,\varepsilon})-\theta_{\rm tr})\mathfrak{a}\cdot(v-\dot\lambda^{\eta,\varepsilon}) + \frac{\alpha}{q}|v|^q + \delta^*_S(v)\,{\rm d}z{\rm d}t + \int_0^s 2\kappa\,((\lambda^{\eta,\varepsilon}-\mathscr{L}(\nabla'_\varepsilon y^{\eta,\varepsilon}), v-\dot\lambda^{\eta,\varepsilon}))_\varepsilon\,{\rm d}t\\ &\quad+\int_0^s\int_\Omega 2\eta\nabla_p\lambda^{\eta,\varepsilon}\cdot\nabla_p v\,{\rm d}z{\rm d}t + \eta\|\nabla_p\lambda_0\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}\\ &\geq \eta\|\nabla_p\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})} + \frac{\eta}{\varepsilon^2}\|\lambda^{\eta,\varepsilon}_{,3}(s)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})} + \int_0^s\int_\Omega \frac{\alpha}{q}|\dot\lambda^{\eta,\varepsilon}|^q + \delta^*_S(\dot\lambda^{\eta,\varepsilon})\,{\rm d}z{\rm d}t. \qquad (42)\end{aligned}$$

Let us take an $s \in [0,T]$ arbitrary but fixed. Then, from (24b), we can choose a further subsequence of ε's *dependent on* s, labeled $\varepsilon_{k(s)}$, such that

$$\frac{1}{{\varepsilon_{k(s)}}^2}\|\lambda^{\eta,\varepsilon_{k(s)}}_{,3}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)})} \to d_s \in \mathbb{R}^{M+1}.$$

Let us work, for the moment, only with this special subsequence and pass to the limit $\varepsilon_{k(s)} \to 0_+$ in (42) to obtain

$$\int_0^s \int_\omega (\Theta(w^\eta) - \theta_{\rm tr})\mathfrak{a} \cdot (v - \dot\lambda^\eta) + \frac{\alpha}{q}|v|^q + \delta_S^*(v)\,\mathrm{d}z_p\mathrm{d}t + \int_0^s 2\kappa(\!(\lambda^\eta - \mathscr{L}(\nabla_p y^\eta|b^\eta), v - \dot\lambda^\eta)\!)_p\,\mathrm{d}t$$
$$+ \int_0^s \int_\omega 2\eta\nabla_p\lambda^\eta \cdot \nabla_p v\,\mathrm{d}z_p\mathrm{d}t + \eta\|\nabla_p\lambda_0\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})}$$
$$\geq \eta\|\nabla_p\lambda^\eta(s)\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})} + \eta d_s + \int_0^s \int_\omega \frac{\alpha}{q}|\dot\lambda^\eta|^q + \delta_S^*(\dot\lambda^\eta)\,\mathrm{d}z_p\mathrm{d}t, \tag{43}$$

for all $v \in L^q(0,T;L^q(\omega;\mathbb{R}^{M+1})) \cap L^\infty(0,T;W^{1,2}(\omega;\mathbb{R}^{(M+1)\times 2}))$.

To see this, we employ (40c) and (41) on the left-hand side to pass to the limit (even for the whole sequence $\varepsilon \to 0_+$) in $\int_0^s \int_\Omega (\Theta(w^{\eta,\varepsilon}) - \theta_{\rm tr})\mathfrak{a} \cdot (v - \dot\lambda^{\eta,\varepsilon})\,\mathrm{d}z\mathrm{d}t$.

Further, let us choose $t \in [0,T]$ arbitrarily but fixed, and denote, for the sake of simplicity, $\Lambda_t^{\eta,\varepsilon} := \lambda^{\eta,\varepsilon}(t) - \mathscr{L}(\nabla'_\varepsilon y^{\eta,\varepsilon}(t))$. Then, the weak convergences (40a)–(40b), shown in Step 1, yield that $\nabla'_\varepsilon y^{\eta,\varepsilon}(t) \to (\nabla_p y^\eta|b^\eta)(t)$ strongly in $L^2(\Omega;\mathbb{R}^{3\times 3})$. Thus, by (D3), Nemytskii continuity and the estimate (24b), we also get that $\Lambda_t^{\eta,\varepsilon} \to \lambda^\eta(t) - \mathscr{L}(\nabla_p y^\eta(t)|b^\eta(t)) =: \Lambda_t^\eta$ strongly in $L^2(\Omega;\mathbb{R}^{M+1})$.

Let us show that in such a case, for $\varepsilon \to 0_+$,

$$\nabla'_\varepsilon \triangle_\varepsilon^{-1}\Lambda_t^{\eta,\varepsilon} \to \nabla_p \triangle_p^{-1}\Lambda_t^\eta \qquad \text{in } L^2(\Omega;\mathbb{R}^{M+1}).$$

Indeed, denote $h_t^\varepsilon = \triangle_\varepsilon^{-1}\Lambda_t^{\eta,\varepsilon}$; then h_t^ε solves

$$\int_\Omega \nabla_p h_t^\varepsilon \cdot \nabla_p \phi + \frac{1}{\varepsilon^2}h^\varepsilon_{t,3}\,\phi_{,3} - \Lambda_t^{\eta,\varepsilon}\phi\,\mathrm{d}z = 0 \qquad \forall \phi \in W_0^{1,2}(\Omega;\mathbb{R}^{M+1}). \tag{44}$$

Taking ϕ independent of z_3 this simplifies to

$$\int_\Omega \nabla_p h_t^\varepsilon \cdot \nabla_p \phi - \Lambda_t^{\eta,\varepsilon}\phi\,\mathrm{d}z = 0 \qquad \forall \phi \in W_0^{1,2}(\omega;\mathbb{R}^{M+1}). \tag{45}$$

Since $\|\nabla_p h_t^\varepsilon\|_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}$ is uniformly bounded (owing to the bounds on $\Lambda_t^{\eta,\varepsilon}$), we pass to the limit $\varepsilon \to 0_+$ in (45) and get that $\nabla_p h_t^\varepsilon \rightharpoonup \nabla_p h_t$ in $L^2(\Omega;\mathbb{R}^{(M+1)\times 2})$ where h_t solves

$$\int_\omega \nabla_p h_t \cdot \nabla_p \phi - \Lambda_t^\eta \phi\,\mathrm{d}z_p = 0 \qquad \forall \phi \in W_0^{1,2}(\omega;\mathbb{R}^{M+1}). \tag{46}$$

Here, we relied on the fact that the limit difference Λ_t^η does not depend on z_3, i.e., $h = \triangle_p^{-1}\Lambda_t^\eta$.

Next, test (44) by $\varepsilon\phi$ and notice that $\frac{1}{\varepsilon}\|h^\varepsilon_{t,3}\|_{L^2(\Omega;\mathbb{R}^{M+1})}$ is uniformly bounded (owing to the bounds on $\Lambda_t^{\eta,\varepsilon}$) to get $\frac{1}{\varepsilon}h^\varepsilon_{t,3} \rightharpoonup 0$ in $L^2(\Omega;\mathbb{R}^{M+1})$. Finally, by testing the difference of (44) and (46) with $h_t^\varepsilon - h_t$, we obtain even that $\nabla'_\varepsilon h_t^\varepsilon \to (\nabla_p h_t|0)$ *strongly* in $L^2(\Omega;\mathbb{R}^{(M+1)\times 3})$. Note that all the above would stay valid even if we had only $\Lambda_t^{\eta,\varepsilon} \rightharpoonup \Lambda_t^\eta$ in $L^2(\Omega;\mathbb{R}^{M+1})$ at hand.

Thus, relying on Lebegue's dominated convergence theorem, we have that

$$\int_0^s 2\kappa(\!(\lambda^{\eta,\varepsilon} - \mathscr{L}(\nabla'_\varepsilon y^{\eta,\varepsilon}), v - \dot\lambda^{\eta,\varepsilon})\!)_\varepsilon\,\mathrm{d}t \to \int_0^s 2\kappa(\!(\lambda^\eta - \mathscr{L}(\nabla_p y^\eta|b^\eta), v - \dot\lambda^\eta)\!)_p\,\mathrm{d}t.$$

Finally, on the left-hand side of (42) in term $\int_0^s \int_\Omega 2\eta\nabla_p\lambda^{\eta,\varepsilon} \cdot \nabla_p v\,\mathrm{d}z\mathrm{d}t$, we use (40d) again combined with Lebegue's dominated convergence; on the right-hand side of (42), we rely on the weak lower semicontinuity of the involved convex terms to obtain (43).

Next, we aim to show that $d_s \equiv 0$. Clearly, $d \geq 0$ and the opposite inequality could be immediately seen if we were allowed to put $v = \dot{\lambda}^\eta$ in (43). Yet, $\dot{\lambda}^\eta$ does not need to have the required regularity. So we introduce a sequence of smooth functions $\{\lambda_\ell^\eta\}_{\ell>0}$ such that $\lambda_\ell^\eta \to \lambda^\eta$ strongly in $W^{1,q}(0,T;L^q(\omega;\mathbb{R}^{M+1}))$ and $\nabla_p\lambda_\ell^\eta(t) \to \nabla_p\lambda^\eta(t)$ strongly in $L^2(\omega;\mathbb{R}^{M+1})$ for $\ell \to 0_+$ for all $t \in [0,T]$. Putting then $v = \dot{\lambda}_\ell^\eta$ in (43) yields

$$\int_0^s\int_\omega (\Theta(w^\eta)-\theta_{\rm tr})\mathfrak{a}\cdot(\dot{\lambda}_\ell^\eta - \dot{\lambda}^\eta) + \frac{\alpha}{q}|\dot{\lambda}_\ell^\eta|^q + \delta_S^*(\dot{\lambda}_\ell^\eta)\,\mathrm{d}z_p\mathrm{d}t + \int_0^s 2\kappa\langle\!\langle\lambda^\eta - \mathscr{L}(\nabla_p y^\eta|b^\eta), \dot{\lambda}_\ell^\eta - \dot{\lambda}^\eta\rangle\!\rangle_p\,\mathrm{d}t$$
$$+ \int_0^s\int_\omega 2\eta\nabla_p\lambda^\eta{\cdot}\nabla_p\dot{\lambda}_\ell^\eta\,\mathrm{d}z_p\mathrm{d}t + \eta\|\nabla_p\lambda_0\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})}$$
$$\geq \eta\|\nabla_p\lambda^\eta(s)\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})} + \eta d_s + \int_0^s\int_\omega \frac{\alpha}{q}|\dot{\lambda}^\eta|^q + \delta_S^*(\dot{\lambda}^\eta)\,\mathrm{d}z_p\mathrm{d}t. \tag{47}$$

Reformulating, by means of by parts integration, $\int_0^s\int_\omega 2\eta\nabla_p\lambda^\eta{\cdot}\nabla_p\dot{\lambda}_\ell^\eta\,\mathrm{d}z_p\mathrm{d}t$ as

$$\int_0^s\int_\omega 2\eta\nabla_p\lambda^\eta{\cdot}\nabla_p\dot{\lambda}_\ell^\eta\,\mathrm{d}z_p\mathrm{d}t = \int_0^s\int_\omega 2\eta(\nabla_p\lambda^\eta - \nabla_p\lambda_\ell^\eta){\cdot}\nabla_p\dot{\lambda}_\ell^\eta\,\mathrm{d}z_p\mathrm{d}t + \int_0^s\int_\Omega 2\eta\nabla_p\lambda_\ell^\eta{\cdot}\nabla_p\dot{\lambda}_\ell^\eta\,\mathrm{d}z_p\mathrm{d}t$$
$$= \int_0^s\int_\omega 2\eta(\nabla_p\lambda^\eta - \nabla_p\lambda_\ell^\eta){\cdot}\nabla_p\dot{\lambda}_\ell^\eta\,\mathrm{d}z_p\mathrm{d}t$$
$$+\eta\big(\|\nabla_p\lambda_\ell^\eta(s)\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})} - \|\nabla_p\lambda_\ell^\eta(0)\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})}\big) \tag{48}$$

and passing to the limit $\ell \to 0_+$ yields that

$$\int_0^s\int_\omega 2\eta\nabla_p\lambda^\eta{\cdot}\nabla_p\dot{\lambda}_\ell^\eta\,\mathrm{d}z_p\mathrm{d}t \to \eta\big(\|\nabla_p\lambda^\eta(s)\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})} - \|\nabla_p\lambda_0\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})}\big).$$

Therefore, passing $\ell \to 0_+$ in (47) gives that $d_s \leq 0$.

Last but not least, note that the s-dependent subsequence $\varepsilon_{k(s)}$ was used to pass at the limit merely in the term $\frac{1}{\varepsilon^2}\|\lambda_{,3}^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)})}$, all other limit passages hold in the whole sequence of ε's. Hence, we arrive at the relation $\frac{1}{\varepsilon_{k(s)}{}^2}\|\lambda_{,3}^{\eta,\varepsilon_{k(s)}}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)})} \to 0$ for all subsequences $\varepsilon_{k(s)}$ in which the left-hand side converges, and, by uniqueness of the limit, we conclude that

$$\frac{1}{\varepsilon^2}\|\lambda_{,3}^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)})} \to 0 \tag{49}$$

in the original sequence of ε's, independently of the chosen $s \in [0,T]$. Thus, we conclude that the normal part of (39d) and (36) hold.

STEP 4: PHASE-FIELD-RELATED ENERGY EQUALITY AND STRONG CONVERGENCE OF $\dot{\lambda}^{\eta,\varepsilon}$. In this step, let us deduce an energy equality that is related to the phase field. To this end, we reformulate the flow rule (16) (exploiting the convexity of $|\cdot|^q$) into the following equivalent form

$$\int_0^s\int_\Omega \alpha|\dot\lambda^{\eta,\varepsilon}|^{q-2}\dot\lambda^{\eta,\varepsilon}\cdot(v-\dot\lambda^{\eta,\varepsilon})+(\Theta(w^{\eta,\varepsilon})-\theta_{\rm tr})\mathfrak{a}\cdot(v-\dot\lambda^{\eta,\varepsilon})+\delta_S^*(v)\,\mathrm{d}z\mathrm{d}t$$
$$+\int_0^s 2\kappa(\!(\lambda^{\eta,\varepsilon}-\mathscr{L}(\nabla'_\varepsilon y^{\eta,\varepsilon}),v-\dot\lambda^{\eta,\varepsilon})\!)_\varepsilon\,\mathrm{d}t+\int_0^s\int_\Omega 2\eta\nabla_p\lambda^{\eta,\varepsilon}\cdot\nabla_p v+\frac{2\eta}{\varepsilon^2}\lambda^{\eta,\varepsilon}_{,3}\cdot v_{,3}\,\mathrm{d}z\mathrm{d}t$$
$$\geq\eta\|\nabla_p\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}-\eta\|\nabla_p\lambda_0\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}+\frac{\eta}{\varepsilon^2}\|\lambda^{\eta,\varepsilon}_{,3}(s)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})}+\int_0^s\int_\Omega\delta_S^*(\dot\lambda^{\eta,\varepsilon})\,\mathrm{d}z\mathrm{d}t \tag{50}$$

and test (50) by $v=0$ to get

$$-\Big(\int_0^s\int_\Omega \alpha|\dot\lambda^{\eta,\varepsilon}|^{q-2}\dot\lambda^{\eta,\varepsilon}\cdot\dot\lambda^{\eta,\varepsilon}+(\Theta(w^{\eta,\varepsilon})-\theta_{\rm tr})\mathfrak{a}\cdot\dot\lambda^{\eta,\varepsilon}\,\mathrm{d}z\mathrm{d}t+\int_0^s 2\kappa(\!(\lambda^{\eta,\varepsilon}-\mathscr{L}(\nabla'_\varepsilon y^{\eta,\varepsilon}),\dot\lambda^{\eta,\varepsilon})\!)_\varepsilon\,\mathrm{d}t\Big)$$
$$\geq\eta\Big(\|\nabla_p\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}-\|\nabla_p\lambda_0\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2}}+\frac{1}{\varepsilon^2}\|\lambda^{\eta,\varepsilon}_{,3}(s)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})}\Big)+\int_0^s\int_\Omega\delta_S^*(\dot\lambda^{\eta,\varepsilon})\,\mathrm{d}z\mathrm{d}t \tag{51}$$

and also by $v=2\dot\lambda^{\eta,\varepsilon}$ to get (if $\dot\lambda^{\eta,\varepsilon}$ does not have the required regularity we can proceed as in Step 3 above, namely we can smoothen $\dot\lambda^{\eta,\varepsilon}$, perform by parts integration analogous to (48) and pass to limit with the mollifying parameter which gives the desired result)

$$\Big(\int_0^s\int_\Omega \alpha|\dot\lambda^{\eta,\varepsilon}|^{q-2}\dot\lambda^{\eta,\varepsilon}\cdot\dot\lambda^{\eta,\varepsilon}+(\Theta(w^{\eta,\varepsilon})-\theta_{\rm tr})\mathfrak{a}\cdot\dot\lambda^{\eta,\varepsilon}\,\mathrm{d}z\mathrm{d}t+\int_0^s 2\kappa(\!(\lambda^{\eta,\varepsilon}-\mathscr{L}(\nabla'_\varepsilon y^{\eta,\varepsilon}),\dot\lambda^{\eta,\varepsilon})\!)_\varepsilon\,\mathrm{d}t\Big)$$
$$+2\eta\Big(\|\nabla_p\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}-\|\nabla_p\lambda_0\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}+\frac{1}{\varepsilon^2}\|\lambda^{\eta,\varepsilon}_{,3}(s)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})}\Big)$$
$$\geq\eta\Big(\|\nabla_p\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}-\|\nabla_p\lambda_0\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}+\frac{1}{\varepsilon^2}\|\lambda^{\eta,\varepsilon}_{,3}(s)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})}\Big)-\int_0^s\int_\Omega\delta_S^*(\dot\lambda^{\eta,\varepsilon})\,\mathrm{d}z\mathrm{d}t,$$

where we relied on the one-homogeneity of $\delta_S^*(\cdot)$. In other words,

$$-\Big(\int_0^s\int_\Omega \alpha|\dot\lambda^{\eta,\varepsilon}|^{q-2}\dot\lambda^{\eta,\varepsilon}\cdot\dot\lambda^{\eta,\varepsilon}+(\Theta(w^{\eta,\varepsilon})-\theta_{\rm tr})\mathfrak{a}\cdot\dot\lambda^{\eta,\varepsilon}\,\mathrm{d}z\mathrm{d}t+\int_0^s 2\kappa(\!(\lambda^{\eta,\varepsilon}-\mathscr{L}(\nabla'_\varepsilon y^{\eta,\varepsilon}),\dot\lambda^{\eta,\varepsilon})\!)_\varepsilon\,\mathrm{d}t\Big)$$
$$\leq\eta\Big(\|\nabla_p\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}-\|\nabla_p\lambda_0\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}+\frac{1}{\varepsilon^2}\|\lambda^{\eta,\varepsilon}_{,3}(s)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})}\Big)+\int_0^s\int_\Omega\delta_S^*(\dot\lambda^{\eta,\varepsilon})\,\mathrm{d}z\mathrm{d}t; \tag{52}$$

combining this with (51), we obtain the *phase-field-related energy equality* in the bulk, more precisely

$$\int_0^s\int_\Omega \alpha|\dot\lambda^{\eta,\varepsilon}|^q\,\mathrm{d}z\mathrm{d}t=-\int_0^s\int_\Omega(\Theta(w^{\eta,\varepsilon})-\theta_{\rm tr})\mathfrak{a}\cdot\dot\lambda^{\eta,\varepsilon}\,\mathrm{d}z\mathrm{d}t-\int_0^s 2\kappa(\!(\lambda^{\eta,\varepsilon}-\mathscr{L}(\nabla'_\varepsilon y^{\eta,\varepsilon}),\dot\lambda^{\eta,\varepsilon})\!)_\varepsilon\,\mathrm{d}t$$
$$-\eta\Big(\|\nabla_p\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}-\|\nabla_p\lambda_0\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}+\frac{1}{\varepsilon^2}\|\lambda^{\eta,\varepsilon}_{,3}(s)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})}\Big)-\int_0^s\int_\Omega\delta_S^*(\dot\lambda^{\eta,\varepsilon})\,\mathrm{d}z\mathrm{d}t. \tag{53}$$

By an analogous procedure, we get from (36) the *phase-field-related energy equality* in the thin film

$$\int_0^s \int_\omega \alpha|\dot{\lambda}^\eta|^q \,\mathrm{d}z_p\mathrm{d}t = -\int_0^s \int_\omega (\Theta(w^\eta) - \theta_{\mathrm{tr}})\mathfrak{a}\cdot\dot{\lambda}^\eta \,\mathrm{d}z_p\mathrm{d}t - \int_0^s 2\kappa\,(\!(\lambda^\eta - \mathscr{L}(\nabla_p y^\eta|b^\eta), \dot{\lambda}^\eta)\!)_p \,\mathrm{d}t$$
$$-\eta\big(\|\nabla_p\lambda^\eta(s)\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})} - \|\nabla_p\lambda_0\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})}\big) - \int_0^s \int_\omega \delta_S^*(\dot{\lambda}^\eta)\,\mathrm{d}z_p\mathrm{d}t. \quad (54)$$

Having (53) and (54) at hand, we prove the *strong* convergences (39c) and the in-plane part of (39d). Indeed, we have

$$\int_0^s \int_\omega \alpha|\dot{\lambda}^\eta|^q \,\mathrm{d}z_p\mathrm{d}t \le \liminf_{\varepsilon\to 0_+} \int_0^s \int_\Omega \alpha|\dot{\lambda}^{\eta,\varepsilon}|^q \,\mathrm{d}z\mathrm{d}t \le \limsup_{\varepsilon\to 0_+} \int_0^s \int_\Omega \alpha|\dot{\lambda}^{\eta,\varepsilon}|^q \,\mathrm{d}z\mathrm{d}t$$
$$\stackrel{\text{(I)}}{=} \limsup_{\varepsilon\to 0_+}\Bigg(-\int_0^s \int_\Omega (\Theta(w^{\eta,\varepsilon}) - \theta_{\mathrm{tr}})\mathfrak{a}\cdot\dot{\lambda}^{\eta,\varepsilon} + \delta_S^*(\dot{\lambda}^{\eta,\varepsilon})\,\mathrm{d}z\mathrm{d}t - \int_0^s 2\kappa\,(\!(\lambda^{\eta,\varepsilon} - \mathscr{L}(\nabla'_\varepsilon y^{\eta,\varepsilon}), \dot{\lambda}^{\eta,\varepsilon})\!)_\varepsilon \,\mathrm{d}t$$
$$+\,\eta\bigg(\|\nabla_p\lambda_0\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})} - \|\nabla_p\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})} - \frac{1}{\varepsilon^2}\|\lambda^{\eta,\varepsilon}_{,3}(s)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})}\bigg)\Bigg)$$
$$\stackrel{\text{(II)}}{=} -\lim_{\varepsilon\to 0_+}\Bigg(\int_0^s\int_\Omega (\Theta(w^{\eta,\varepsilon}) - \theta_{\mathrm{tr}})\mathfrak{a}\cdot\dot{\lambda}^{\eta,\varepsilon}\,\mathrm{d}z\mathrm{d}t + \int_0^s 2\kappa\,(\!(\lambda^{\eta,\varepsilon} - \mathscr{L}(\nabla'_\varepsilon y^{\eta,\varepsilon}), \dot{\lambda}^{\eta,\varepsilon})\!)_\varepsilon\,\mathrm{d}t + \frac{\eta}{\varepsilon^2}\|\lambda^{\eta,\varepsilon}_{,3}(s)\|^2_{L^2(\Omega;\mathbb{R}^{M+1})}\Bigg)$$
$$+\,\eta\big(\|\nabla_p\lambda_0\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})} - \liminf_{\varepsilon\to 0_+}\|\nabla_p\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})}\big) - \liminf_{\varepsilon\to 0_+}\int_0^s\int_\Omega \delta_S^*(\dot{\lambda}^{\eta,\varepsilon})\,\mathrm{d}z\mathrm{d}t$$
$$\stackrel{\text{(III)}}{=}\le -\int_0^s \int_\omega (\Theta(w^\eta) - \theta_{\mathrm{tr}})\mathfrak{a}\cdot\dot{\lambda}^\eta\,\mathrm{d}z_p\mathrm{d}t - \int_0^s 2\kappa\,(\!(\lambda^\eta - \mathscr{L}(\nabla_p y^\eta|b^\eta), \dot{\lambda}^\eta)\!)_p\,\mathrm{d}t$$
$$\|\nabla_p\lambda_0\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})} - \|\nabla_p\lambda^\eta(s)\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})} - \int_0^s\int_\omega \delta_S^*(\dot{\lambda}^\eta)\,\mathrm{d}z_p\mathrm{d}t$$
$$\stackrel{\text{(IV)}}{=} \int_0^s\int_\omega \alpha|\dot{\lambda}^\eta|^q\,\mathrm{d}z_p\mathrm{d}t,$$

where the inequalities on the first line follow from the weak lower semicontinuity of the norm and a general lim inf $\le$ lim sup relation, the equality (I) is due to (53), the equality (II) follows from general lim sup, lim inf relation, the inequality (III) was obtained by lower semicontinuity of the convex terms and (40c) and (40d), the limit $\varepsilon \to 0_+$ uses (41), (49) and similar techniques as when passing to the limit in the flow rule in *Step 3*. Finally, (IV) is due to (54).

So, we conclude that $\|\dot{\lambda}^{\eta,\varepsilon}\|_{L^q(Q;\mathbb{R}^{M+1})} \to \|\dot{\lambda}^\eta\|_{L^q(Q;\mathbb{R}^{M+1})}$ and, as the space $L^q(Q;\mathbb{R}^{M+1})$ is uniformly convex, also

$$\dot{\lambda}^{\eta,\varepsilon} \to \dot{\lambda}^\eta \qquad \text{in } L^q(Q;\mathbb{R}^{M+1}). \quad (55)$$

Moreover, using (55) and passing to the limit $\varepsilon \to 0_+$ in (53) and comparing to (54) yields that

$$\|\nabla_p\lambda^{\eta,\varepsilon}(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})} \to \|\nabla_p\lambda^\eta(s)\|^2_{L^2(\Omega;\mathbb{R}^{(M+1)\times 2})} \qquad \forall s \in [0,T]. \quad (56)$$

STEP 5: THIN-FILM SEMI-STABILITY. Fix again some $t \in [0,T]$ arbitrarily. Then, we test (14) (formulated only in the deformation-related energy) by $\tilde{y}^\varepsilon_\delta(z) := \tilde{y}(z_p) + \varepsilon z_3 b_\delta(z_p)$ with some arbitrary $\tilde{y} \in W^{2,2}(\omega;\mathbb{R}^3)$ and a smooth approximation $\{b_\delta\}_{\delta>0}$ of an arbitrary $\tilde{b} \in W^{1,2}(\omega;\mathbb{R}^3)$ (the smoothing is required in order to obtain the test function in $W^{2,2}(\Omega;\mathbb{R}^3))$ such that $\tilde{y}(z_p)+\varepsilon z_3 b_\delta(z_p)=0$ a.e. on $\Gamma_{\rm D}$. Then, by taking first $\liminf_{\varepsilon\to 0}$ then $\liminf_{\delta\to 0_+}$ one arrives to

$$\begin{aligned}\mathfrak{G}_\eta(t) &\le \liminf_{\varepsilon\to 0_+}\mathfrak{G}^\varepsilon_\eta(t)\\ &\le \lim_{\delta\to 0_+}\left(\liminf_{\varepsilon\to 0_+}\mathfrak{G}^\varepsilon_\eta(t,\bar{y}^\varepsilon_\delta,\lambda^{\eta,\varepsilon}(t))+\int_\Omega \eta\left|\nabla'_\varepsilon\bar{y}^\varepsilon_\delta-\nabla'_\varepsilon y^{\eta,\varepsilon}(t)\right|\,\mathrm{d}z\right)\\ &\le \lim_{\delta\to 0_+}\left(\limsup_{\varepsilon\to 0_+}\mathfrak{G}^\varepsilon_\eta(t,\bar{y}^\varepsilon_\delta,\lambda^{\eta,\varepsilon}(t))+\int_\Omega \eta\left|\nabla'_\varepsilon\bar{y}^\varepsilon_\delta-\nabla'_\varepsilon y^{\eta,\varepsilon}(t)\right|\,\mathrm{d}z\right)\\ &= \mathfrak{G}_\eta(t,\tilde{y},\tilde{b},\lambda^\eta(t))+\int_\omega \eta\left|(\nabla_p\tilde{y}|\tilde{b})-(\nabla_p y^\eta(t)|b^\eta(t))\right|\,\mathrm{d}z_p,\end{aligned}$$

where we used (39c), (39d) and the compact embedding $L^q(\Omega;\mathbb{R}^{M+1})\Subset W^{-1,2}(\Omega;\mathbb{R}^{M+1})$ (recall that $q\ge 2$) to pass to the limit in $\mathfrak{G}^\varepsilon_\eta(t,\bar{y}^\varepsilon_\delta,\lambda^{\eta,\varepsilon}(t))$ while (40a), (40b) was used to pass to the limit in $\int_\Omega \eta\left|\nabla'_\varepsilon\bar{y}^\varepsilon_\delta-\nabla'_\varepsilon y^{\eta,\varepsilon}(t)\right|\,\mathrm{d}z$. Observe that this is equivalent to (33).

Moreover, letting $\tilde{y}:=y^\eta(t)$ and $\tilde{b}:=b^\eta(t)$ yields

$$\lim_{\varepsilon\to 0_+}\mathfrak{G}^\varepsilon_\eta(t)=\mathfrak{G}_\eta(t)\qquad \text{for all } t\in[0,T]. \tag{57}$$

From this we may, similarly as in [11], deduce that

$$\begin{aligned}\nabla^2_p y^{\eta,\varepsilon}(t)&\to\nabla^2_p y^\eta(t)\quad \text{in } L^2(\Omega;\mathbb{R}^{3\times 2\times 2}),\\ \nabla_p\frac{1}{\varepsilon}y^{\eta,\varepsilon}_{,3}(t)&\to\nabla_p b^\eta(t)\quad \text{in } L^2(\Omega;\mathbb{R}^{3\times 2}),\\ \frac{1}{\varepsilon^2}y^{\eta,\varepsilon}_{,33}(t)&\to 0\quad \text{in } L^2(\Omega;\mathbb{R}^3),\end{aligned}$$

thus showing (39a)–(39b). As we will not need this improved convergence in the following, we omit a detailed proof.

STEP 6: THIN- FILM DEFORMATION- RELATED ENERGY EQUALITY. We show the deformation-related energy equality (34) as two inequalities. One follows from the bulk inequality by taking $\liminf_{\varepsilon\to 0_+}$ with the aid of the convergences (39a)–(39d), the data qualification (D2) as

$$\begin{aligned}&\mathfrak{G}_\eta(T)-\mathfrak{G}_\eta(0)+\eta\mathrm{Var}_{|\cdot|}(\nabla_p y^\eta|b^\eta)\\ &\le\liminf_{\varepsilon\to 0_+}\left(\mathfrak{G}^\varepsilon_\eta(T)-\mathfrak{G}^\varepsilon_\eta(0)+\eta\mathrm{Var}_{|\cdot|}(\nabla'_\varepsilon y^{\eta,\varepsilon})\right)\\ &\le\limsup_{\varepsilon\to 0_+}\int_0^T[\mathfrak{G}^\varepsilon_\eta]'_t(t)+\left\langle[\mathfrak{G}^\varepsilon_\eta]'_\lambda(t),\dot{\lambda}^{\eta,\varepsilon}(t)\right\rangle\,\mathrm{d}t\\ &\le\int_0^T[\mathfrak{G}_\eta]'_t(t)+\left\langle[\mathfrak{G}_\eta]'_\lambda(t),\dot{\lambda}^\eta(t)\right\rangle\,\mathrm{d}t\end{aligned}\tag{58}$$

as far as the first inequality is concerned, recall that $\mathrm{Var}_{|\cdot|}$ is lower-semicontinuous under the convergences (39a)–(39b).

The opposite inequality is a consequence of the thin-film semi-stability (33) (cf. [24,30,42] and [8] for an analogous (and more detailed) proof as the one given below). To see this, we introduce a partition of $[0,T]$, $0=t_0<t_1<\cdots<t_{N(\beta)}=T$, such that $\max\{|t^\beta_{i-1}-t^\beta_i|:\ i=1,\ldots,N(\beta)\}\le\beta$ and test (33) at the time t^β_{i-1} by $(y^\eta(t^\beta_i),b^\eta(t^\beta_i))$, $i=1,\ldots,N(\beta)$. Summing from 0 to $N(\beta)$ reveals that

$$\mathfrak{G}_\eta(T) - \mathfrak{G}_\eta(0) + \eta \mathrm{Var}_{|\cdot|}(\nabla_p y^\eta | b^\eta) \geq \sum_{i=1}^{N(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} [\mathfrak{G}_\eta]'_t(t, y^\eta(t_i^\beta))\,\mathrm{d}t + \sum_{i=1}^{N(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} \left\langle [\mathfrak{G}_\eta]'_\lambda(y^\eta(t_i^\beta), b^\eta(t_i^\beta), \lambda^\eta(t)), \dot\lambda^\eta(t) \right\rangle \mathrm{d}t, \tag{59}$$

where

$$\sum_{i=1}^{N(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} \left\langle [\mathfrak{G}_\eta]'_\lambda(y^\eta(t_i^\beta), b^\eta(t_i^\beta), \lambda^\eta(t)), \dot\lambda^\eta(t) \right\rangle dt = 2\kappa \sum_{i=1}^{N(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} ((\lambda^\eta(t) - \mathscr{L}(\nabla_p y^\eta(t_i^\beta) | b^\eta(t_i^\beta)), \dot\lambda^\eta(t)))_p \, dt$$
$$+ \underbrace{\sum_{i=1}^{N(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} ((\lambda^\eta(t) - \lambda^\eta(t_i^\beta), \dot\lambda^\eta))_p \, dt}_{\text{(i)}} + \underbrace{\sum_{i=1}^{N(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} ((\lambda^\eta(t_i^\beta) - \mathscr{L}(\nabla_p y^\eta(t_i^\beta) | b^\eta(t_i^\beta)), \dot\lambda^\eta(t_i^\beta)))_p \, dt}_{\text{(ii)}}$$
$$+ \underbrace{\sum_{i=1}^{N(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} ((\dot\lambda^\eta(t_i^\beta) - \mathscr{L}(\nabla_p y^\eta(t_i^\beta) | b^\eta(t_i^\beta)), \dot\lambda^\eta(t) - \dot\lambda^\eta(t_i^\beta)))_p \, dt}_{\text{(iii)}} \tag{60}$$

To make the limit passage for $\beta \to 0_+$, one makes use of the fact (cf. [16]) that for every Bochner integrable $h\colon [0,T] \to X$, with X a Banach space, there is a sequence of partitions of $[0,T]$ such that h can be approached by its piecewise constant interpolants h_β defined on $[0,T]$ as $h_\beta|_{[t_{i-1}^\beta, t_i^\beta)} := h(t_i^\beta)$, $i = 1, \ldots, N(\beta)$ strongly to h in $L^1(0,T;X)$; more precisely

$$\lim_{\beta \to 0_+} \sum_{i=1}^{N(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} \|h_\beta(t) - h(t)\|_X \, \mathrm{d}t = 0.$$

Hence, one may assume that we always take partitions for which this approximation result holds and we may assume that

$$\lambda_\beta^\eta \rightharpoonup \lambda^\eta \quad \text{in } L^q(0,T; L^q(\omega; \mathbb{R}^{M+1})), \tag{61a}$$
$$y_\beta^\eta \rightharpoonup y^\eta \quad \text{in } L^p(0,T; W^{1,p}(\omega; \mathbb{R}^3)), \tag{61b}$$
$$b_\beta^\eta \rightharpoonup b^\eta \quad \text{in } L^2(0,T; L^2(\omega; \mathbb{R}^3)), \tag{61c}$$
$$\dot\lambda_\beta^\eta \to \dot\lambda^\eta \quad \text{in } L^1(0,T; L^q(\omega; \mathbb{R}^{M+1})), \tag{61d}$$
$$\left[((\lambda^\eta - \mathscr{L}(\nabla_p y^\eta | b^\eta), \dot\lambda^\eta))_p\right]_\beta \to ((\lambda^\eta - \mathscr{L}(\nabla_p y^\eta | b^\eta), \dot\lambda^\eta))_p \quad \text{in } L^1(0,T). \tag{61e}$$

Using (61b) we establish that $\sum_{i=1}^{N(\beta)} \int_{t_{i-1}^\beta}^{t_i^\beta} [\mathfrak{G}_\eta]'_t(t, y^\eta(t_i^\beta))\,\mathrm{d}t \to \int_0^T [\mathfrak{G}_\eta]'_t(t, y^\eta(t))\,\mathrm{d}t$; moreover, (61a) assures that (i) in (60) converges to 0, by (61e) we immediately see that (ii) in (60) converges to $\int_0^T ((\lambda^\eta - \mathscr{L}(\nabla_p y^\eta | b^\eta), \dot\lambda^\eta))_p \,\mathrm{d}t$ and, finally, by the uniform boundedness of $\dot\lambda^\eta(t_i^\beta) - \mathscr{L}(\nabla_p y^\eta(t_i^\beta) | b^\eta(t_i^\beta))$ in $L^\infty(0,T; W^{-1,2}(\omega; \mathbb{R}^{M+1}))$ and (61d) the term (iii) in (60) converges to 0.

Thus, we got that

$$\mathfrak{G}_\eta^\varepsilon(T) - \mathfrak{G}_\eta^\varepsilon(0) + \eta \mathrm{Var}_{|\cdot|}(\nabla'_\varepsilon y^{\eta,\varepsilon}) \geq \int_0^T [\mathfrak{G}_\eta]'_t(t) + \big\langle [\mathfrak{G}_\eta]'_\lambda(t), \dot{\lambda}^\eta(t)\big\rangle \,\mathrm{d}t$$

and combining this with (58) as well as (57) we obtain that

$$\mathrm{Var}_{|\cdot|}(\nabla'_\varepsilon y^{\eta,\varepsilon}) \to \mathrm{Var}_{|\cdot|}(\nabla_p y^\eta | b^\eta) \tag{62}$$

STEP 7: THIN- FILM ENTHALPY EQUATION. Recall that the bulk enthalpy equation reads as

$$\int_Q \mathscr{K}(\lambda^{\eta,\varepsilon}, w^{\eta,\varepsilon}) \nabla'_\varepsilon w^{\eta,\varepsilon} \cdot \nabla'_\varepsilon \zeta - w^{\eta,\varepsilon} \dot{\zeta} \,\mathrm{d}z\mathrm{d}t + \int_\Sigma \mathfrak{b}\Theta(w^{\eta,\varepsilon})\zeta \,\mathrm{d}S\mathrm{d}t$$
$$= \int_Q \big(\delta_S^*(\dot{\lambda}^{\eta,\varepsilon}) + \alpha|\dot{\lambda}^{\eta,\varepsilon}|^q + \Theta(w^{\eta,\varepsilon})\mathfrak{a} \cdot \dot{\lambda}^{\eta,\varepsilon}\big)\zeta \,\mathrm{d}z\mathrm{d}t + \eta \int_{\overline{Q}} \zeta \mathscr{H}_\varepsilon(\,\mathrm{d}x\mathrm{d}t)$$
$$+ \int_\Omega w_0^{\eta,\varepsilon} \zeta(0) \,\mathrm{d}z + \int_\Sigma \mathfrak{b}\theta_{\mathrm{ext}} \zeta \,\mathrm{d}S\mathrm{d}t \tag{63}$$

with $\bar{\zeta} \in C^1(\overline{\mathscr{Q}})$ and $\bar{\zeta}(T) = 0$. Let us restrict ourselves to test functions independent of z_3. When taking $\varepsilon \to 0_+$ in (63), we aim to get (37).

First, let us show that

$$\lim_{\varepsilon\to 0_+} \int_{\overline{Q}} \zeta \mathscr{H}_\varepsilon^\eta(\mathrm{d}z\mathrm{d}t) = \int_{\overline{Q}} \zeta \mathscr{H}^\eta(\mathrm{d}z\mathrm{d}t). \tag{64}$$

To this end, recall that from the a-priori estimates, (23) follows the existence of a limit measure $\overline{\mathscr{H}}$ such that

$$\mathscr{H}_\varepsilon^\eta \overset{*}{\rightharpoonup} \overline{\mathscr{H}} \quad \text{in } \mathscr{M}(\overline{Q}), \tag{65}$$

while, on the other hand, (62) ensures that

$$\lim_{\varepsilon\to 0} \mathscr{H}_\varepsilon^\eta(\overline{Q}) = \mathscr{H}^\eta(\overline{Q}). \tag{66}$$

Now, the contradiction argument in [42, Proposition 4.3] supports that (65)–(66) indeed yield (64). More precisely, if, by contradiction, it held that $\mathscr{H}^\eta \neq \overline{\mathscr{H}}$, we could define the Borel set $\mathfrak{B} := \mathrm{supp}\,(\mathscr{H}^\eta - \overline{\mathscr{H}}) \subset \overline{Q}$ and (66) would imply that

$$\int_{\mathfrak{B}} (\mathscr{H}^\eta - \overline{\mathscr{H}}) \,\mathrm{d}z\mathrm{d}t > 0$$

(otherwise (66) would be violated), which immediately contradicts the weak* lower semicontinuity of the map $\varepsilon \mapsto \int_{\mathfrak{B}} \mathscr{H}_\varepsilon^\eta(\,\mathrm{d}z\mathrm{d}t)$.

For the other terms in (63), we use $\lambda^{\eta,\varepsilon} \to \lambda^\eta$ in $L^q(0,T; L^q(\Omega; \mathbb{R}^{M+1}))$, $w^{\eta,\varepsilon} \to w^\eta$ in $L^s(0,T; L^s(\Omega))$, for any $1 \leq s < 5/3$; the latter convergence ensures also that $w^{\eta,\varepsilon} \to w^\eta$ in $L^1(0,T; L^1(\Sigma))$ which allows us to pass to the limit in the boundary terms on the left-hand side of (63) as well as that $\mathscr{K}(\lambda^{\eta,\varepsilon}, w^{\eta,\varepsilon}) \to \mathscr{K}(\lambda^\eta, w^\eta)$ in $L^\beta(0,T; L^\beta(\Omega; \mathbb{R}^{3\times 3}))$ for any $1 \leq \beta < +\infty$. Hence, we obtain (37). ◻

5 Relaxation in the microscopic thin-film model

In this section, we surpass scales to rigorously obtain the mesoscopic model formally given by (10a)–(10c).

As mentioned in Sect. 2, this upscaling lets the interfacial energy vanish; this may lead to fast spatial oscillations of the deformation gradient, on one hand, as well as of the Cosserat vector, on the other hand. A standard tool to capture these oscillations is the theory of (gradient) *Young measures* [29,37,51].

Let $\mathscr{O} \subset \mathbb{R}^l$ be a Lebesgue measurable subset with finite measure. Young measures are weakly measurable and essentially bounded mappings $\nu \in L^1(\mathscr{O}; C_0(\mathbb{R}^d))^* \cong L^\infty_{\mathrm{w}}(\mathscr{O}; \mathscr{M}(\mathbb{R}^d))$; here, $C_0(\mathbb{R}^d)$ denotes the space of continuous functions on $\mathbb{R}^d$ vanishing at infinity, so that $\mathscr{M}(\mathbb{R}^d)$ denotes the space of Radon measures on $\mathbb{R}^d$. Having a bounded sequence $\{u_k\}_{k\in\mathbb{N}} \subset L^p(\mathscr{O}; \mathbb{R}^d)$ for $1 \le p < +\infty$ then there is a subsequence (not relabeled) and a Young measure ν such that $\lim_{k\to\infty} \int_{\mathscr{O}} h(x, u_k(x))\,\mathrm{d}x = \int_{\mathscr{O}} \int_{\mathbb{R}^d} h(x, F)\,\nu_x(\mathrm{d}F)\mathrm{d}x$ whenever $\{h(\cdot, u_k)\}_{k\in\mathbb{N}} \subset L^1(\mathscr{O})$ is uniformly integrable, where $h : \mathscr{O} \times \mathbb{R}^d \to \mathbb{R}$ is a Carathéodory integrand. We then say that ν is generated by $\{u_k\}_{k\in\mathbb{N}}$. The set of mappings from $L^\infty_{\mathrm{w}}(\mathscr{O}; \mathscr{M}(\mathbb{R}^d))$ generated by bounded sequences in $L^p(\mathscr{O}; \mathbb{R}^d)$ is denoted by $\mathscr{Y}^p(\mathscr{O}; \mathbb{R}^d)$.

An important subset of $\mathscr{Y}^p(\mathscr{O}; \mathbb{R}^d)$ is the set of so-called p-gradient Young measures ($1 < p < +\infty$) which consists of measures generated by $\{\nabla y_k\}_{k\in\mathbb{N}}$ of a bounded sequence of mappings $\{y_k\}_{k\in\mathbb{N}} \subset W^{1,p}(\mathscr{O}; \mathbb{R}^d)$. The set of p-gradient Young measures (shortly gradient Young measures) is denoted by $\mathscr{G}^p(\mathscr{O}; \mathbb{R}^{d\times l})$. Occasionally, we may write $\mathscr{G}^p_{\gamma_{\mathrm{D}}}(\mathscr{O}; \mathbb{R}^{d\times l})$ to indicate that $y_k = 0$ on $\gamma_{\mathrm{D}} \subset \partial\mathscr{O}$.

Further, we use the shorthand notation (momentum operator) "$\bullet$" defined through

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

Denoting $\mathrm{id} : \mathbb{R}^{d\times l} \to \mathbb{R}^{d\times l}$ the identity mapping, we speak of $\mathrm{id}\bullet\nu$ as the *mean value* of the gradient Young measure $\nu \in \mathscr{G}^p(\mathscr{O}; \mathbb{R}^{d\times l})$. It can be proved, cf. [29], that whenever $\nu \in \mathscr{G}^p(\mathscr{O}; \mathbb{R}^{d\times l})$ there exists $y \in W^{1,p}(\mathscr{O}; \mathbb{R})$ such that $\nabla y = \mathrm{id}\bullet\nu$ a.e. on $\mathscr{O}$. Additionally, ν is an element of $\mathscr{G}^p_{\gamma_{\mathrm{D}}}(\mathscr{O}; \mathbb{R}^{d\times l})$ if and only if $y = 0$ on γ_{D}.

5.1 Weak formulation

Let us now state the weak formulation of (10a)–(10c).

Definition 3 We call the quintuple $(y, \nu, \mu, \lambda, w)$, where

$$y \in B(0, T; W^{1,p}(\omega; \mathbb{R}^3)), \tag{67a}$$

$$\nu \in (\mathscr{G}^p_{\gamma_{\mathrm{D}}}(\omega; \mathbb{R}^{3\times 2}))^{[0,T]}, \tag{67b}$$

$$\mu \in (\mathscr{Y}^p(\omega; \mathbb{R}^3))^{[0,T]}, \tag{67c}$$

$$\lambda \in W^{1,q}(0, T; L^q(\mathbb{R}^{M+1})), \tag{67d}$$

$$w \in L^\infty(0, T; L^1(\omega)), \tag{67e}$$

such that $y(t) = \mathrm{id}\bullet\nu_{z_p}(t)$ for a.a. $z_p \in \omega$ and all $t \in [0, T]$ a weak solution of (10a)–(10c) if it satisfies

1. Minimization property:
$$\mathscr{G}(t, y(t), \nu(t), \mu(t), \lambda(t), \Theta(w(t))) \le \mathscr{G}(t, \bar{y}, \bar{\nu}, \bar{\mu}, \lambda(t), \Theta(w(t))) \tag{68}$$
for every $(\bar{y}, \bar{\nu}, \bar{\mu}) \in W^{1,p}(\omega; \mathbb{R}^3) \times \mathscr{G}^p_{\gamma_{\mathrm{D}}}(\omega; \mathbb{R}^{3\times 2}) \times \mathscr{Y}^p(\omega; \mathbb{R}^3)$ such that $\bar{y} = \mathrm{id}\bullet\bar{\nu}_{z_p}$ for almost all $z_p \in \omega$ and $\mathscr{G}$ defined in (9).
2. Flow rule:
$$\int_0^T 2\kappa\langle\!\langle \lambda - \mathscr{L}\bullet(\nu, \mu), v - \dot{\lambda}\rangle\!\rangle_p \,\mathrm{d}t + \int_0^T\int_\omega (\Theta(w^{\eta,\varepsilon}) - \theta_{\mathrm{tr}})\mathfrak{a}\cdot(v - \dot{\lambda}) + \frac{\alpha}{q}|v|^q + \delta^*_S(v)\,\mathrm{d}z_p\mathrm{d}t$$
$$\ge \int_0^T\int_\omega \frac{\alpha}{q}|\dot{\lambda}|^q + \delta^*_S(\dot{\lambda})\,\mathrm{d}z_p\mathrm{d}t \tag{69}$$
for all test functions $v \in L^q(0, T; L^q(\omega; \mathbb{R}^{M+1}))$.

3. ENTHALPY EQUATION:

$$\int_{\mathscr{Q}} \mathscr{K}(\lambda, w)\nabla_p w\cdot\nabla_p \zeta - w\dot{\zeta}\,\mathrm{d}z_p\mathrm{d}t + \int_0^T\int_{\partial\omega} \mathfrak{b}\Theta(w)\zeta\,\mathrm{d}S_p\mathrm{d}t$$

$$= \int_{\mathscr{Q}} \big(\delta_S^*(\dot{\lambda}) + \alpha|\dot{\lambda}|^q + (\Theta(w))\mathfrak{a}\cdot\dot{\lambda}\big)\zeta\,\mathrm{d}z_p\mathrm{d}t + \int_\omega w_0\zeta(0)\,\mathrm{d}z_p + \int_0^T\int_{\partial\omega} \mathfrak{b}\theta_{\mathrm{ext}}\zeta\,\mathrm{d}S_p\mathrm{d}t \tag{70}$$

for every $\zeta \in C^1(\overline{\mathscr{Q}})$ such that $\zeta(T) = 0$.

4. REMAINING INITIAL CONDITIONS:

$$\nu_{z_p}(0) = \delta_{y_{0,0}(z_p)}, \qquad \mu_{z_p}(0) = \delta_{b_0(z_p)}, \qquad \lambda(0) = \lambda_{0,0}, \tag{71}$$

with $y_{0,0}(z_p)$, $b_0(z_p)$ and $\lambda_{0,0}$ referring to (38).

Notice that in this formulation, we used the (not completely standard) notation $B(0, T; X)$ for the space of function $[0, T] \mapsto X$, X a Banach space, that are bounded but not necessarily Lebesgue measurable. Also, we used the notation

$$\Psi\bullet(\nu,\mu)(z_p) := \int_{\mathbb{R}^{3\times 2}}\int_{\mathbb{R}^3} \Psi(A|b)\,\mathrm{d}\nu_{z_p}(A)\,\mathrm{d}\mu_{z_p}(b),$$

with Ψ a continuous function with at most p-growth.

Remark 6 (*Deformation-related energy equality*) Note that we omit a deformation-related energy equality analogous to (34). Since we scale down the rate-independent dissipation due to $\eta|(\nabla_p\dot{y}^\eta|b^\eta)|$ to zero, such an equality is a direct consequence of (68) and, hence, becomes redundant. To see this, we may proceed as Step 6 of the proof of Theorem 1 and introduce a partition of the interval $[0, T]$, $0 = t_0^\beta \le t_1^\beta \dots t_{K(\beta)}^\beta = T$ and test (68) at $t = t_{i-1}^\beta$ by $(y(t_i^\beta), \nu(t_i^\beta), \mu(t_i^\beta))$; summing and passing to the limit $\beta \to 0$ leads, as in Step 6 of the proof of Theorem 1, to the inequality

$$\mathfrak{G}(T) - \mathfrak{G}(0) \ge \int_0^T \mathfrak{G}_t'(t) + \big\langle \mathfrak{G}_\lambda'(t), \dot{\lambda}(t)\big\rangle\,\mathrm{d}t, \tag{72}$$

where

$$\mathfrak{G}(t) = \mathfrak{G}(t, y(t), \nu(t), \mu(t), \lambda(t)) := \int_\omega W\bullet(\nu,\mu)\,\mathrm{d}z_p + \kappa\|\lambda - \mathscr{L}\bullet(\nu,\mu)\|^2_{W^{-1,2}(\omega;\mathbb{R}^{3\times3})}$$
$$- \int_\omega f^0\cdot y\,\mathrm{d}z_p - \int_{\gamma_\mathrm{N}} g^0\cdot y\,\mathrm{d}S_p, \tag{73}$$

is the deformation-related part of the mesoscopic Gibbs free energy.

The other inequality is then obtained by an analogous procedure. We test the Eq. (68) at $t = t_i^\beta$ by $(y(t_{i-1}^\beta), \nu(t_{i-1}^\beta), \mu(t_{i-1}^\beta))$. We obtain an "energy-related" inequality because the dissipation component related to $\eta|(\nabla_p\dot{y}^\eta|b^\eta)|$ is not present in (68) anymore.

5.2 Existence of weak solutions

Theorem 2 *Let $\{(y^\eta, b^\eta, \lambda^\eta, w^\eta)\}_{\eta>0}$ be a family of weak solutions of the thin-film problem (8a)–(8c) as found in Theorem 1. Then, there exists a quintuple $(y, \nu, \mu, \lambda, w)$, satisfying (67), and a sequence $\eta \to 0_+$ such that*

$$\lambda^\eta \to \lambda \quad in\ W^{1,q}(0,T;L^q(\omega;\mathbb{R}^{M+1})), \tag{74}$$

and

$$w^\eta \rightharpoonup w \quad in\ L^r(0,T;W^{1,r}(\omega)),\ for\ every\ r < \frac{5}{4}, \tag{75a}$$

$$w^\eta \to w \quad in\ L^s(0,T;L^s(\omega)),\ for\ every\ s < \frac{5}{3}. \tag{75b}$$

Moreover, for each $t \in [0,T]$, there exists a subsequence $\eta_{k(t)}$ such that $\nabla y_{\eta_{k(t)}}(t)$ generates a gradient Young measure $\nu(t)$, $y_{\eta_{k(t)}}(t) \rightharpoonup y(t)$ in $W^{1,p}(\omega;\mathbb{R}^3)$ and $b_{\eta_{k(t)}}(t)$ generates a Young measure $\mu(t)$.

At least one cluster point found in this way is then a weak solution to (10a)–(10c) in the sense of Definition 3.

Proof For lucidity, let us divide the proof into several steps. Let us note that the idea of the proof, in particular the technique of selecting a suitable cluster point, roughly follows [8].

Step 1: Selection of subsequences and reformulation of the flow rule. Similarly as in Step 1 of the proof of Theorem 1, we choose, owing to the a-priori estimates (24)–(25) (and the Aubin–Lions theorem), a (not relabeled) subsequence of $\eta \to 0_+$ and find (λ, w) such that

$$\lambda^\eta \rightharpoonup \lambda \quad \text{in } W^{1,q}(0,T;L^q(\omega;\mathbb{R}^{M+1})) \tag{76}$$

and (75) hold as well as the limit $\lim_{\eta\to 0_+} \mathfrak{G}_\eta(T)$ is well defined. Recall that, again as in Step 1 in the proof of Theorem 1, we have the additional convergences $\lambda^\eta(t) \rightharpoonup \lambda(t)$ in $L^q(\omega;\mathbb{R}^{M+1})$ for all $t \in [0,T]$ and $\Theta(w^\eta) \to \Theta(w)$ in $L^{q'}(\mathcal{Q})$.

Now, let us turn our attention to the flow rule (36), more specifically to the penalty term

$$\int_0^T 2\kappa (\!(\lambda^\eta(t) - \mathscr{L}(\nabla_p y^\eta(t)|b^\eta(t)), v - \dot\lambda^\eta)\!)_p \,\mathrm{d}t \tag{77}$$

involved in $\int_0^T \langle [\mathscr{G}_\eta]'_t, v - \dot\lambda^\eta\rangle \,\mathrm{d}t$, which turns out to be the most troublesome. Indeed, note that since the limit for $(\nabla y^\eta, b^\eta)$ is evaluated pointwise in $t \in [0,T]$, the limit of $\mathscr{L}(\nabla_p y^\eta(t)|b^\eta(t))$ (taken again pointwise) is not guaranteed to be measurable in time. Moreover, $\dot\lambda^\eta$ converges only weakly in $L^q(\mathcal{Q};\mathbb{R}^{M+1})$, and, thus, convergence of this term for a.a. $t \in [0,T]$ cannot be expected. To handle the latter obstacle, we plug the energy equality (34) into (36) with $s = T$ to obtain a weaker *reformulated flow rule*:

$$\begin{aligned}
&\mathfrak{G}_\eta(T) + \eta \mathrm{Var}_{|\cdot|}(\nabla_p y^\eta|b^\eta) + \eta\|\nabla_p\lambda^\eta(T)\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})} + \int_{\mathcal{Q}} \frac{\alpha}{q}|\dot\lambda^\eta|^q + \delta^*_S(\dot\lambda^\eta)\,\mathrm{d}z_p\mathrm{d}t \\
&\quad\le \mathfrak{G}_\eta(0) + \int_0^T [\mathfrak{G}_\eta]'_t(t, y^\eta(t))\,\mathrm{d}t + \int_{\mathcal{Q}} (\Theta(w^\eta) - \theta_{\mathrm{tr}})\mathfrak{a}\cdot(\tilde v - \dot\lambda^\eta) + 2\eta\nabla_p\lambda^\eta\cdot\nabla_p\tilde v + \frac{\alpha}{q}|\tilde v|^q + \delta^*_S(\tilde v)\,\mathrm{d}z_p\mathrm{d}t \\
&\qquad + \int_0^T 2\kappa(\!(\lambda^\eta - \mathscr{L}(\nabla_p y^\eta|b^\eta), \tilde v)\!)_p\,\mathrm{d}t + \eta\|\nabla_p\lambda_0\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})}.
\end{aligned} \tag{78}$$

Indeed, the term $\int_0^T 2\kappa(\!(\lambda^\eta(t) - \mathscr{L}(\nabla_p y^\eta(t)|b^\eta(t)), \dot\lambda)\!)_p\,\mathrm{d}t$ is no longer present in (78).

Further, inspired by [8,16,24], we define

$$\mathfrak{P}^v(t) = \limsup_{\eta\to 0} 2\kappa(\!(\lambda^\eta(t) - \mathscr{L}(\nabla_p y^\eta(t)|b^\eta(t)), v(t))\!)_p \quad \text{and} \quad \mathscr{F}(t) = \limsup_{\eta\to 0}[\mathfrak{G}_\eta]'_t(t, y^\eta(t))$$

for any $v \in L^q(\mathscr{Q};\mathbb{R}^{M+1})$ and every $t \in [0,T]$; notice that both $\mathfrak{P}^v$ and $\mathscr{F}$ are measurable. Moreover, by Fatou's lemma, we have

$$\int_0^T \mathfrak{P}^v(t)\,\mathrm{d}t \ge \limsup_{\eta\to 0_+} \int_0^T 2\kappa\langle\!\langle \lambda^\eta(t) - \mathscr{L}(\nabla_p y^\eta(t)|b^\eta(t)), v(t)\rangle\!\rangle_p\,\mathrm{d}t,$$
$$\int_0^T \mathscr{F}(t)\,\mathrm{d}t \ge \limsup_{\eta\to 0_+} \int_0^T [\mathfrak{G}_\eta]'_t(t, y^\eta(t))\,\mathrm{d}t.$$

Since $L^q(\mathscr{Q};\mathbb{R}^{M+1})$ is separable, we consider, for now, the test functions $v = v^\ell$ only from a countable dense subset of $L^q(\mathscr{Q};\mathbb{R}^{M+1})$, denoted by $\mathscr{V}$. Next, we fix $t \in [0,T]$ and choose a subsequence of η's labeled η_{t,v^ℓ} such that

$$\mathfrak{P}^{v^\ell}(t) = \lim_{\eta_{t,v^\ell}\to 0_+} 2\kappa\langle\!\langle \lambda^{\eta_{t,v^\ell}}(t) - \mathscr{L}(\nabla_p y^{\eta_{t,v^\ell}}(t)|b^{\eta_{t,v^\ell}}(t)), v^\ell(t)\rangle\!\rangle_p, \tag{79a}$$
$$\mathscr{F}(t) = \lim_{\eta_{t,v^\ell}\to 0_+} [\mathfrak{G}_\eta]'_t\big(t, y^{\eta_{t,v^\ell}}(t)\big). \tag{79b}$$

By a diagonal selection, we can find a further subsequence labeled η_t such that (79) holds for all v^ℓ. Note that the chosen subsequence remains to be time-dependent.

Now, owing to the a-priori estimates (23b) and (23c), we choose yet another subsequence of $\eta_{k(t)}$ (not relabeled) such that $\{\nabla_p y_{\eta_{k(t)}}(t)\}_{k\in\mathbb{N}}$ generates the gradient Young measure $\nu_{z_p}(t)$ and $\{b_{\eta_{k(t)}}(t)\}_{k\in\mathbb{N}}$ generates the Young measure $\mu_{z_p}(t)$; so,

$$\mathfrak{P}^v(t) = \lim_{\eta_{k(t)}\to 0_+} 2\kappa\langle\!\langle \lambda^{\eta_{k(t)}}(t) - \mathscr{L}(\nabla_p y^{\eta_{k(t)}}(t)|b^{\eta_{k(t)}}(t)), v(t)\rangle\!\rangle_p\,\mathrm{d}t = 2\kappa\langle\!\langle \lambda(t) - \mathscr{L}\bullet(\nu,\mu), v(t)\rangle\!\rangle_p,$$
$$\mathscr{F}(t) = \lim_{\eta_{k(t)}\to 0_+} [\mathfrak{G}_\eta]'_t(t, y_{\eta_{k(t)}}(t)) = \mathfrak{G}'_t(t, y(t)).$$

Thus, when passing to the limit $\eta \to 0_+$ in (78), using weak lower semicontinuity of the convex terms and non-negativity of $\eta\mathrm{Var}_{|\cdot|}(\nabla_p y^\eta|b^\eta) + \eta\|\nabla_p\lambda^\eta(T)\|^2_{W^{-1,2}(\omega;\mathbb{R}^{(M+1)\times 2})}$ we get, similarly as in Step 3 of the proof of Theorem 1, the reformulated mesoscopic flow rule

$$\mathfrak{G}(T) + \int_{\mathscr{Q}} \frac{\alpha}{q}|\dot\lambda|^q + \delta_S^*(\dot\lambda)\,\mathrm{d}z_p\mathrm{d}t \le \mathfrak{G}(0) + \int_0^T \mathfrak{G}'_t(t, y(t))\,\mathrm{d}t$$
$$+ \int_{\mathscr{Q}} (\Theta(w) - \theta_{\mathrm{tr}})\mathfrak{a}\cdot(v - \dot\lambda) + \frac{\alpha}{q}|v|^q + \delta_S^*(v)\,\mathrm{d}z_p\mathrm{d}t + \int_0^T 2\kappa\langle\!\langle \lambda - \mathscr{L}\bullet(\nu,\mu), v\rangle\!\rangle_p\,\mathrm{d}t, \tag{80}$$

where, by density, the test functions can be taken from the whole space $L^q(\mathscr{Q};\mathbb{R}^{M+1})$.

STEP 2: MINIMIZATION PRINCIPLE, BACK TO THE ORIGINAL FLOW RULE. First, we notice that (68) is equivalent to

$$\mathfrak{G}(t, y, \nu, \mu, \lambda(t)) \le \mathfrak{G}(t, \bar y, \bar\nu, \bar\mu, \lambda(t))$$

for every $(\bar y, \bar\nu, \bar\mu) \in W^{1,p}(\omega;\mathbb{R}^3) \times \mathscr{G}^p_{\Gamma_D}(\omega;\mathbb{R}^{3\times 2}) \times \mathscr{Y}^p(\omega;\mathbb{R}^3)$ such that $\bar y = \mathrm{id}\bullet\bar\nu_{z_p}$ for a.a. $z_p \in \omega$.

Thus, thanks to (33), we have

$$\mathfrak{G}(t, y, \nu, \mu, \lambda(t)) \le \liminf_{\eta_{k(t)}\to 0_+} \mathfrak{G}_{\eta_{k(t)}}(t, y^{\eta_{k(t)}}(t), b^{\eta_{k(t)}}(t), \lambda^{\eta_{k(t)}}(t))$$
$$\le \liminf_{\eta_{k(t)}\to 0_+} \mathfrak{G}_{\eta_{k(t)}}(t, \tilde y, \tilde b, \lambda^{\eta_{k(t)}}(t)) + \int_\omega \eta_{k(t)}|(\nabla_p y^{\eta_{k(t)}}(t)|b^{\eta_{k(t)}}(t)) - (\nabla_p\tilde y|\tilde b)|\,\mathrm{d}z_p$$
$$= \int_\omega W(\nabla_p\tilde y|\tilde b)\,\mathrm{d}z_p + \kappa\|\lambda(t) - \mathscr{L}(\nabla_p\tilde y|\tilde b)\|^2_{W^{-1,2}(\omega;\mathbb{R}^{M+1})} - \int_\omega f^0\cdot\tilde y\,\mathrm{d}z_p - \int_{\gamma_{\mathrm{N}}} g^0\cdot\tilde y\,\mathrm{d}S_p$$

for every $\tilde{y} \in W^{2,2}(\omega;\mathbb{R}^3)$ and $\tilde{b} \in W^{1,2}(\omega;\mathbb{R}^3)$, such that $y = 0$ on γ_D. By density, we have that

$$\mathfrak{G}(t, y, \nu, \mu, \lambda(t)) \le \int_\omega W(\nabla_p\tilde{y}|\tilde{b})\,\mathrm{d}z_p + \kappa\|\lambda(t) - \mathscr{L}(\nabla_p\tilde{y}|\tilde{b})|^2_{W^{-1,2}(\omega;\mathbb{R}^{M+1})} - \int_\omega f^0\cdot\tilde{y}\,\mathrm{d}z_p - \int_{\gamma_N} g^0\cdot\tilde{y}\,\mathrm{d}S_p$$

even for all $\tilde{y} \in W^{1,2}(\omega;\mathbb{R}^3)$ satisfying $y = 0$ on γ_D and all $\tilde{b} \in L^2(\omega;\mathbb{R}^3)$. Take an arbitrary pair of admissible Young measure $(\tilde{\nu},\tilde{\mu}) \in \mathscr{G}^p_{\gamma_D}(\omega;\mathbb{R}^{3\times 2}) \times \mathscr{Y}^p(\Omega;\mathbb{R}^3)$, then we can always find its bounded generating sequence $\{(\nabla_p\tilde{y}_k, \tilde{b}_k)\}_{k\in\mathbb{N}} \subset L^p(\omega;\mathbb{R}^{3\times 2}) \times L^p(\omega;\mathbb{R}^3)$ such that $\{|\nabla_p\tilde{y}_k|^p + |\tilde{b}_k|^p\}_{k\in\mathbb{N}}$ is equi-integrable [23], the sequence $\{y_k\}_{k\in\mathbb{N}} \subset W^{1,p}(\omega;\mathbb{R}^3)$ is bounded and $y_k(z_1, z_2) = 0$ for $z \in \gamma_D$ for all $k \in \mathbb{N}$. Passing to the limit for $k \to \infty$ in the previous inequality with $\tilde{y}_k$ and $\tilde{b}_k$ in place of $\tilde{y}$ and $\tilde{b}$ we get that $\mathfrak{G}(t, y, \nu, \mu, \lambda(t)) \le \mathfrak{G}(t, \tilde{y}, \tilde{\nu}, \tilde{\mu}, \lambda(t))$ where $\tilde{y}$ is the weak limit of $\tilde{y}_k$. Hence, Eq. (68) is shown.

Note that as a side product of the above procedure we obtained also that

$$\mathfrak{G}(0) := \mathfrak{G}(0, y(0), \nu(0), \mu(0), \lambda(0)) = \lim_{\eta\to 0_+} \mathfrak{G}_\eta(0), \tag{81a}$$

$$\mathfrak{G}(T) := \mathfrak{G}(T, y(T), \nu(T), \mu(T), \lambda(T)) = \lim_{\eta\to 0_+} \mathfrak{G}_\eta(T). \tag{81b}$$

Hence, the reformulated flow rule reads as

$$\mathfrak{G}(T) + \int_{\mathscr{Q}} \frac{\alpha}{q}|\dot{\lambda}|^q + \delta^*_S(\dot{\lambda})\,\mathrm{d}z_p\mathrm{d}t \le \mathfrak{G}(0) + \int_0^T \mathfrak{G}'_t(t, y(t))\,\mathrm{d}t$$
$$+ \int_{\mathscr{Q}} (\Theta(w) - \theta_{\mathrm{tr}})\mathfrak{a}\cdot(v - \dot{\lambda}) + \frac{\alpha}{q}|v|^q + \delta^*_S(v)\,\mathrm{d}z_p\mathrm{d}t + \int_0^T 2\kappa(\!(\lambda - \mathscr{L}\bullet(\nu,\mu), v)\!)_p\,\mathrm{d}t, \tag{82}$$

and exploiting the balance of the mesoscopic deformation-related energy equality—cf. Remark 6 and (73)—we also get the *mesoscopic flow rule* (69).

Step 3: Strong convergence of $\dot{\lambda}^\eta$. This convergence is obtained from the monotonicity properties of the dissipation term $|\cdot|^q$ in the reformulated flow rule. Indeed, let us rewrite (78) (relying on the convexity of $|\cdot|^q$) as

$$\mathfrak{G}_\eta(T) + \eta\mathrm{Var}_{|\cdot|}(\nabla_p y^\eta|b^\eta) + \eta\|\nabla_p\lambda^\eta(T)\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})} + \int_{\mathscr{Q}} \delta^*_S(\dot{\lambda}^\eta)\,\mathrm{d}z_p\mathrm{d}t \le \int_0^T [\mathfrak{G}_\eta]'_t(t, y^\eta(t))\,\mathrm{d}t$$
$$+\mathfrak{G}_\eta(0) + \int_{\mathscr{Q}} \alpha|\dot{\lambda}^\eta|^{q-2}\dot{\lambda}^\eta\cdot(\tilde{v} - \dot{\lambda}^\eta) + (\Theta(w^\eta) - \theta_{\mathrm{tr}})\mathfrak{a}\cdot(\tilde{v} - \dot{\lambda}^\eta) + \delta^*_S(\tilde{v}) + 2\eta\nabla_p\lambda^\eta\cdot\nabla_p\tilde{v}\,\mathrm{d}z_p\mathrm{d}t$$
$$+ \int_0^T 2\kappa(\!(\lambda^\eta - \mathscr{L}(\nabla_p y^\eta|b^\eta), \tilde{v})\!)_p\,\mathrm{d}t + \eta\|\nabla_p\lambda_0\|^2_{L^2(\omega;\mathbb{R}^{(M+1)\times 2})}; \tag{83}$$

similarly, (82) is rewritten as

$$\mathfrak{G}(T) + \int_{\mathscr{Q}} \frac{\alpha}{q}|\dot{\lambda}|^q + \delta^*_S(\dot{\lambda})\,\mathrm{d}z_p\mathrm{d}t \le \mathfrak{G}(0) + \int_0^T \mathfrak{G}'_t(t, y(t))\,\mathrm{d}t + \int_0^T 2\kappa(\!(\lambda - \mathscr{L}\bullet(\nu,\mu), v)\!)_p\,\mathrm{d}t$$
$$+ \int_{\mathscr{Q}} \alpha|\dot{\lambda}|^{q-2}\dot{\lambda}\cdot(v - \dot{\lambda}) + (\Theta(w) - \theta_{\mathrm{tr}})\mathfrak{a}\cdot(v - \dot{\lambda}) + \delta^*_S(v)\,\mathrm{d}z_p\mathrm{d}t. \tag{84}$$

Then, having a sequence $\{\lambda'_j\}_{j\in\mathbb{N}} \subset \mathscr{V} \cap C(0,T; W^{1,2}(\omega;\mathbb{R}^{M+1}))$ such that $\lambda'_j \to \dot{\lambda}$ in $L^q(\mathscr{Q};\mathbb{R}^{M+1})$ for $j \to \infty$ (recall that $\mathscr{V}$ is the dense countable subset of $L^q(\mathscr{Q};\mathbb{R}^{M+1})$ used in Step 1), let us test (84) by $\dot{\lambda}^\eta$

and, symmetrically, (83) by λ'_j, as $\dot\lambda$ does not have the required smoothness to be used as a test function in (83) and, moreover, we wish to use (79) (as well as the resulting convergences in Step 1) which is only available for test functions from $\mathscr{V}$.

Let us add (83) and (84) and apply $\lim_{j\to\infty}\limsup_{\eta\to 0}$ to get

$$\alpha\lim_{\eta\to0}\Big(\|\dot\lambda^\eta\|^{q-1}_{L^q(\mathscr{Q};\mathbb{R}^{M+1})}-\|\dot\lambda\|^{q-1}_{L^q(\mathscr{Q};\mathbb{R}^{M+1})}\Big)\Big(\|\dot\lambda^\eta\|_{L^q(\mathscr{Q};\mathbb{R}^{M+1})}-\|\dot\lambda\|_{L^q(\mathscr{Q};\mathbb{R}^{M+1})}\Big)$$
$$\le\limsup_{\eta\to0}\ \alpha\int_0^T\!\!\int_\omega\Big(|\dot\lambda^\eta|^{q-2}\dot\lambda^\eta-|\dot\lambda|^{q-2}\dot\lambda\Big)\cdot(\dot\lambda^\eta-\dot\lambda)\,\mathrm{d}z_p\mathrm{d}t$$
$$\le\lim_{j\to\infty}\limsup_{\eta\to0}\Big(\mathfrak{G}(0)-\mathfrak{G}(T)+\underbrace{\mathfrak{G}_\eta(0)-\mathfrak{G}_\eta(T)}_{\text{(I)}}-\eta\,\underbrace{\mathrm{Var}_{|\cdot|}(\nabla_p y^\eta|b^\eta)}_{\text{(II)}_1}+\eta\int_\omega|\nabla_p\lambda_0|^2-\underbrace{|\nabla_p\lambda^\eta(T)|^2}_{\text{(II)}_2}\,\mathrm{d}z_p$$
$$+\int_0^T\mathfrak{G}'_t(t,y)+\underbrace{[\mathfrak{G}_\eta]'_t(t,y^\eta)}_{\text{(III)}}\,\mathrm{d}t+\int_{\mathscr{Q}}\alpha\,\underbrace{|\dot\lambda^\eta|^{q-2}\dot\lambda^\eta(\lambda'_j-\dot\lambda)+\delta^*_S(\lambda'_j)-\delta^*_S(\dot\lambda)}_{\text{(IV)}}\,\mathrm{d}z_p\mathrm{d}t$$
$$+\int_0^T\underbrace{2\kappa(\!(\lambda^\eta-\mathscr{L}(\nabla_p y^\eta|b^\eta),\lambda'_j)\!)_p}_{\text{(V)}}+\underbrace{2\kappa(\!(\lambda-\mathscr{L}\bullet(\nu,\mu),\dot\lambda^\eta)\!)_p}_{\text{(VI)}}\,\mathrm{d}t$$
$$+\int_{\mathscr{Q}}\underbrace{(\Theta(w^\eta)-\theta_{\mathrm{tr}})(\lambda'_j-\dot\lambda^\eta)+(\Theta(w)-\theta_{\mathrm{tr}})(\dot\lambda^\eta-\dot\lambda)\,\mathrm{d}z\mathrm{d}t}_{\text{(VII)}}+\underbrace{2\eta\nabla_p\lambda^\eta\cdot\nabla_p\lambda'_j}_{\text{(VIII)}}\,\mathrm{d}z_p\mathrm{d}t\Big)$$
$$\le 2\mathfrak{G}(0)-2\mathfrak{G}(T)+\int_0^T 2\mathfrak{G}'_t(t,y)+4\kappa(\!(\lambda-\mathscr{L}\bullet(\nu,\mu),\dot\lambda)\!)_p\,\mathrm{d}t=0.$$

Here, the first inequality is due to Hölder's inequality. Further, we used that term (I) is not smaller than $\mathfrak{G}(0)-\mathfrak{G}(T)$ by (81) and the non-negativity of (II)_1 and (II)_2. The convergence of the term between them to 0 is obvious. Term (III) is, owing to Step 1, bounded from above by $\mathfrak{G}'_t(t,y)$. Now, as $j\to\infty$ term (IV) converges to 0 as $\dot\lambda^\eta$ is bounded uniformly in $L^q(\mathscr{Q};\mathbb{R}^{M+1})$. The limsup of the term (V), again by Step 1, is bounded from above by $(\!(\lambda-\mathscr{L}\bullet(\nu,\mu),\dot\lambda)\!)_p$; for the terms (VI) and (VII) we proceed analogously as in Step 1, while the term (VIII) converges to 0 as the limit $\eta\to0_+$ is executed first.

Finally, note that the last equality is due to the balance of the deformation-related energy; cf. Remark 6. Hence, we obtained $\|\dot\lambda^\eta\|_{L^q(\mathscr{Q};\mathbb{R}^{M+1})}\to\|\dot\lambda\|_{L^q(\mathscr{Q};\mathbb{R}^{M+1})}$ and from (76) by the uniform convexity of $L^q(\mathscr{Q};\mathbb{R}^{M+1})$ also (74).

Step 4: Enthalpy equation. It only remains to prove the enthalpy equation (70); to obtain it, we pass to the limit $\eta\to0_+$ in (37) following ideas of Step 7 in the proof of Theorem 1. In order to pass to the limit in the terms expressing the heating due to dissipation, however, we need to show that $\eta\int_{\bar Q}\zeta\,\mathscr{H}^\eta(\mathrm{d}z_p\mathrm{d}t)\to0$. To see this, we actually need only to show that $\lim_{\eta\to0}\eta\mathrm{Var}_{|\cdot|}(\nabla_p y^\eta|b^\eta)=0$ which we obtain by passing to the limit in (34). Indeed,

$$\limsup_{\eta\to0}\eta\mathrm{Var}_{|\cdot|}(\nabla_p y^\eta|b^\eta)$$
$$\le\limsup_{\eta\to0}\Big(-\mathfrak{G}_\eta(T)+\mathfrak{G}_\eta(0)+\int_0^T\big\langle[\mathfrak{G}_\eta]'_\lambda(y^\eta(t),b^\eta(t),\lambda^\eta(t)),\dot\lambda^\eta\big\rangle+[\mathfrak{G}_\eta]'_t(t,y^\eta(t))\,\mathrm{d}t\Big).\qquad(85)$$

To pass to the limit on the right-hand side, we rewrite

$$\big\langle[\mathfrak{G}_\eta]'_\lambda(y^\eta(t),b^\eta(t),\lambda^\eta(t)),\dot\lambda^\eta\big\rangle=\big\langle[\mathfrak{G}_\eta]'_\lambda(y^\eta(t),b^\eta(t),\lambda^\eta(t)),\dot\lambda\big\rangle+\big\langle[\mathfrak{G}_\eta]'_\lambda(y^\eta(t),\lambda^\eta(t)),\dot\lambda^\eta-\dot\lambda\big\rangle.\quad(86)$$

Note that for the first term we get by Step 1 (if necessary, we can approximate $\dot{\lambda}$ by $\{\dot{\lambda}_\ell\}_{\ell\in\mathbb{N}}$ belonging to the dense countable subset of $L^q(\mathscr{Q};\mathbb{R}^{M+1})$ used in Step 1)

$$\left\langle [\mathfrak{G}_\eta]'_\lambda(y^\eta(t), b^\eta(t), \lambda^\eta(t)), \dot{\lambda}\right\rangle \le \int_0^T \left\langle \mathfrak{G}'_\lambda(\nu(t), \mu(t), \lambda(t)), \dot{\lambda}\right\rangle \mathrm{d}t, \tag{87}$$

while the second term converges to 0 in $L^1([0,T])$ owing to Step 3. Thus, we get

$$0 \le \limsup_{\eta\to 0_+} \eta \mathrm{Var}_{|\cdot|}(\nabla_p y^\eta | b^\eta) \le \mathfrak{G}(0) - \mathfrak{G}(T) + \int_0^T \left\langle \mathfrak{G}'_\lambda(\nu(t), \mu(t), \lambda(t)), \dot{\lambda}\right\rangle + \mathfrak{G}'_t(t, y(t))\,\mathrm{d}t \le 0, \tag{88}$$

where the last inequality follows from Remark 6. □

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Chapter 3

Computer modelling of static martensitic thin films

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Modelling of Thin Films of Shape-Memory Alloys

G. Pathó

After a brief introduction to the physical and mathematical problem related—not only—to shape-memory alloys and a review of different variational models for thin martensitic films, a numerical approach based on the first laminate is proposed, followed by computational experiments.

1 Introduction

Shape-memory alloys (SMAs) have been subject to extensive theoretical and experimental research since the last half a century—when the martensitic phase transformation was first explained in the AuCd alloy in 1951.

This non-diffusive, solid-to-solid phase transformation leads to a change in the crystallographic structure of the material. The SMAs exist in two phases: at high temperature the austenite phase (having one crystallographic configuration with high symmetry—usually cubic structure) while lower temperatures lead to a low-symmetric grid, e.g., tetragonal, orthorhombic, monoclinic, which is then called martensite phase and may occur in M different variants (here $M = 3, 6, 12$ for the cases mentioned above).

Shape-memory alloys belong to the group of intelligent materials: they do not only have the ability to detect changes of their environment—stress and temperature, in particular—but they are also able to react to these changes. Furthermore, this behaviour being induced by the mere transformation of the crystallographic lattice of the alloy, the size of an SMA component can be reduced significantly—up to the order of $10\ \mu m$—without affecting its functionality.

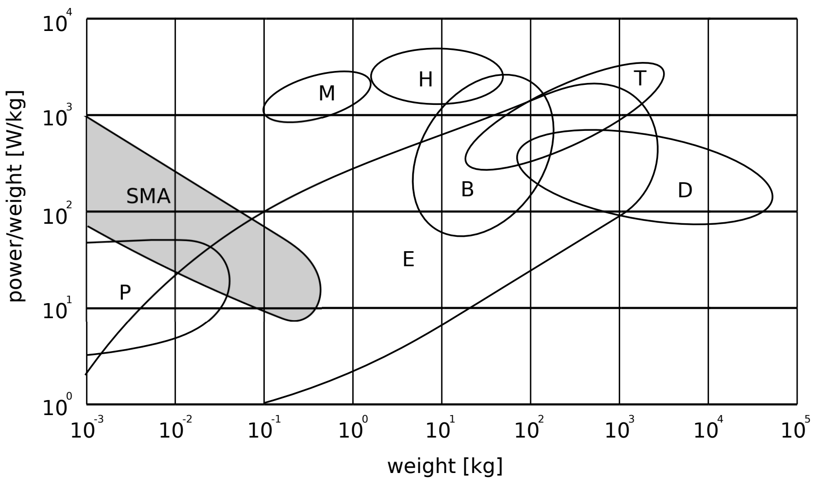

Figure 1: Power–weight ratio for different types of actuators; P – piezoelectric transducers, E – electromotors, M – modeller motors, H – hydraulic motors, B – piston gas-engines, D – piston diesel-engines, T – internalcombustion turbines, SMA - shape-memory alloy actuators (picture in accordance with Figure 6 of Šittner and Novák (2002))

Due to this delicate feature, miniature components made of shape-memory alloys have found numerous applications in many different areas of science and technology from microrobotics to thin films—particularly the sputter-deposited NiTi thin films, which are widely used as microactuators in the micro-electro-mechanical systems (MEMS), e.g., cantilevers, diaphragms, micropumps, microvalves, dumpers (cf. Pan and Cho (2007) for the demonstration of such a dumper), different grippers, springs or mirror actuators. For an extensive overview of the modern decomposition techniques, key engineering characteristics and applications of NiTi thin films cf. Miyazaki et al. (2009).

2 Mathematical Model of SMA Static Problems in 3D

In what follows L^p will denote the standard Lebesgue space of measurable mappings which are integrable with the p-th power for $1 \le p < +\infty$ or essentially bounded for $p = +\infty$. Further, $W^{k,p}$ will stand for the Sobolev space of mappings belonging together with their derivatives up to the order k to L^p.

Usually, the formulation of the mathematical minimization problem related to the static description of bulk shape-memory alloys at a given temperature θ is

$$\begin{aligned} &\text{Minimize} \quad \mathcal{I}(y) = \int_\Omega \varphi(\nabla y(x))\,\mathrm{d}x \\ &\text{subject to} \quad y \in \mathfrak{A}_{y_0}, \end{aligned} \tag{1}$$

where y is the deformation of the reference configuration $\Omega \subset \mathbb{R}^3$, Ω open bounded domain, furthermore, the set $\mathfrak{A}_{y_0} := \{w \in W^{1,p}(\Omega, \mathbb{R}^3) : \det \nabla w > 0 \text{ a.e. in } \Omega,\ w|_{\Gamma_0} = y_0\}$ denotes the set of admissible deformations with $1 < p < +\infty$ and y_0 defining a suitable Dirichlet boundary condition on a prescribed $\Gamma_0 \subset \partial\Omega$, meas$(\Gamma_0) > 0$ such that $\mathfrak{A}_{y_0} \neq \emptyset$.

The Helmholtz free energy density $\varphi\colon \mathbb{R}^{3\times 3} \to \mathbb{R}$ is a continuous function defined on the set of real 3×3 matrices obliging the physical property of material frame-indifference, more precisely

$$\varphi(QF) = \varphi(F) \qquad \forall Q \in SO(3), \tag{2}$$

where $SO(3) = \{Q \in \mathbb{R}^{3\times 3} :\ Q^T Q = QQ^T = I,\ \det Q = 1\}$ denotes the set of all rotations and I the 3×3 identity matrix.

Without loss of generality let us consider the energy density normalized, so that $\varphi \ge 0$. Then different variants of the particular phases are modelled through the multi-well structure of φ, i.e.,

$$\varphi(F) = 0 = \min_{\mathfrak{A}_{y_0}} \varphi(\cdot) \quad \Leftrightarrow \quad F \in \mathcal{A} \cup \mathcal{M}, \tag{3}$$

where $\mathcal{A} := SO(3)U_0$, resp. $\mathcal{M} := SO(3)U_1 \cup SO(3)U_2 \cup \cdots \cup SO(3)U_M$ stands for all the matrices related to the austenitic phase, resp. the martensitic phase (consisting of M variants)—bearing in mind the frame-indifference of the stored energy density, too—the particular matrices U_0, resp. $U_1, \ldots U_M$ are then the so called Bain matrices of the austenite, resp. martensite.

Furthermore, the energy density should satisfy the growth condition

$$c(|A|^p - 1) \le \varphi(A) \le C(1 + |A|^p) \qquad \forall A \in \mathbb{R}^{3\times 3} \tag{4}$$

for some $c, C \in \mathbb{R}$.

Due to the multi-well character of φ—implying its lack of quasiconvexity—(1) may not admit any solution in the class of Sobolev spaces as for any minimizing sequence is allowed to—and does for certain conditions on y_0 and between U_i—develop finer and finer oscillations between the wells.

Let us recall that a function $g\colon \mathbb{R}^{m\times n} \to \mathbb{R}$ is quasiconvex if the inequality

$$g(A) \le \frac{1}{|\mathcal{O}|} \int_{\mathcal{O}} g(A + \nabla\psi(x))\,\mathrm{d}x \tag{5}$$

holds valid for any $A \in \mathbb{R}^{m\times n}$ and any $\psi\colon \mathcal{O} \to \mathbb{R}^m$ smooth, where $\mathcal{O} \subset \mathbb{R}^n$ is an open domain (in fact, the property of quasiconvexity is independent of the chosen domain $\mathcal{O}$).

Two procedures have been proposed to overcome the aforementioned problem of non-existence of classical Sobolev minimizers to (1). Dacorogna (1989) showed that one can extend the functional $\mathcal{I}$ to a relaxed functional $\mathcal{I}_Q$

which defines a minimization problem delicately related to the initial one but exhibiting a solution in the related Sobolev space, cf. the last paragraph, the first equality in (10), in particular. Let us recall that the relaxed problem is connected to the quasiconvexification of φ, namely

$$\begin{aligned} &\text{Minimize} \quad \mathcal{I}_Q(y) = \int_\Omega Q\varphi(\nabla y(x))\,\mathrm{d}x \\ &\text{subject to} \quad y \in \mathfrak{A}_{y_0}, \end{aligned} \tag{6}$$

where $Q\varphi$ is the quasiconvex envelope of the energy density, i.e.,

$$Q\varphi = \sup\{\psi\colon \psi \le \varphi,\ \psi \text{ quasiconvex}\}. \tag{7}$$

The other method for introducing a meaningful solution of (1) stems from extending the notion of solution to the objects called gradient Young measures, which are weakly* measurable mappings $x \mapsto \mu_x\colon \Omega \to \text{rca}(\mathbb{R}^{3\times 3})$—i.e., the mapping $\Omega \to \mathbb{R}\colon x \mapsto \langle \mu_x, v\rangle = \int_{\mathbb{R}^{3\times 3}} v(s)\mu_x(\mathrm{d}s)$ is Lebesgue measurable for every continuous function with compact support $v \in C_0(\mathbb{R}^{3\times 3})$—with values in probability measures generated by sequences of gradients of Sobolev maps.

Then defining the set of all gradient Young measures $\mathcal{G}^p$ as

$$\mathcal{G}^p(\Omega;\mathbb{R}^{3\times 3}) = \left\{\mu \in L^\infty_w(\Omega;\text{rca}(\mathbb{R}^{3\times 3})) : \exists\{y_k\}_{k\in\mathbb{N}} \text{ bounded in } W^{1,p}(\Omega;\mathbb{R}^3) \text{ such that } \delta_{\nabla y_k} \overset{*}{\rightharpoonup} \mu\right\}, \tag{8}$$

where δ_x is the usual delta function with support at the point x and the weak* convergence is understood in the dual space $L^\infty_w(\Omega;\text{rca}(\mathbb{R}^{3\times 3})) \simeq L^1(\Omega; C_0(\mathbb{R}^{3\times 3}))^*$—the subscript w indicating the above mentioned weak* convergence of measures—, one is led to formulate the relaxed minimization problem as

$$\begin{aligned} &\text{Minimize} \quad \mathcal{I}_Y(\mu) = \int_\Omega \int_{\mathbb{R}^{3\times 3}} \varphi(s)\mu_x(\mathrm{d}s)\,\mathrm{d}x \\ &\text{subject to} \quad \mu \in \mathcal{G}^p(\Omega;\mathbb{R}^{3\times 3}), \\ &\qquad\qquad\quad y_\mu \in \mathfrak{A}_{y_0}, \end{aligned} \tag{9}$$

where $y_\mu \in W^{1,p}(\Omega;\mathbb{R}^3)$—called the underlying deformation of the measure μ—is the weak limit of the generating sequence $\{y_k\}_{k\in\mathbb{N}}$ from definition (8).

It can be shown—among others—that

$$\min(6) = \inf(1) = \min(9), \tag{10}$$

whereas any minimizer $y \in \mathfrak{A}_{y_0}$ of (6) admits a minimizing sequence of (1) converging weakly to y in $W^{1,p}(\Omega;\mathbb{R}^3)$ and every minimizer of (9) is generated by gradients of minimizing sequences of (1). The advantage of the Young-measure approach lies in its ability of capturing the microstructure beyond the macroscopic deformation as well. For further details cf. e.g. Dacorogna (1989); Müller (1999); Pedregal (1997); Roubíček (1997).

3 Dimension Reduction

3.1 Limiting Energy Densities

Modelling of thin films of shape-memory alloys relies on a Γ-convergence procedure when going to zero with the material thickness $h > 0$ of the domain $\Omega_h = \omega \times (-h/2, h/2)$, $\omega \subset \mathbb{R}^2$ open and bounded. In order to do so one transforms the total energy $I_h(y)$ to a scaled integral of a reference configuration $\Omega_1 = \omega \times I$, $I := (-1/2, 1/2)$, not depending on h by a scaling factor of $1/h$; cf. Friesecke et al. (2006) for a hierarchy of different nonlinear plate theories arising from different scaling of the free energy and the power of external forces.

More precisely, one is looking for the variational limit

$$\lim_{h\to 0_+} I_h(y) = \lim_{h\to 0_+} \frac{1}{h}\int_{\omega\times I} \varphi\Big(\nabla_p y(x)\Big|\frac{1}{h}\nabla_3 y(x)\Big)\,\mathrm{d}x, \tag{11}$$

where the expressions $\nabla_p y \in \mathbb{R}^{3\times 2}$, resp. $\nabla_3 y \in \mathbb{R}^3$ denote the planar gradient of y, i.e., the gradient of $y = y(x_p)$, $x_p = (x_1, x_2)$, resp. the partial derivative of $y = y(x)$ in the direction e_3 perpendicular to the basis $\{e_1, e_2\}$ of the film ω; the notation $(A|a_3)$ for a 3×2 matrix A with columns a_1 and a_2 means then the 3×3 matrix $\sum_{i=1}^{3} a_i \otimes e_i$.

The first rigorous results were due to Le Dret and Raoult (1995) who obtained the limit functional

$$\mathcal{I}_{\mathcal{LDR}}(y) = \int_\omega Q\varphi_0(\nabla_p y)\,\mathrm{d}x_p, \tag{12}$$

which involved $Q\varphi_0$ the quasiconvex envelope of the effective energy density φ_0 defined for $F \in \mathbb{R}^{3\times 2}$ as

$$\varphi_0(F) = \min_{z\in\mathbb{R}^3} \varphi(F|z), \tag{13}$$

capturing well the average macroscale deformation of the material but with the obvious drawback of losing the finer scale oscillations of the deformation gradient forming the structure of laminates.

For this purpose gradient Young measures introduced above should be taken into account when determining the Γ–limit of the total energy functionals. Freddi and Paroni (2004) arrived at the following expression

$$\mathcal{I}_{\mathcal{FP}}(\mu) = \int_\omega \int_{\mathbb{R}^{3\times 2}} \varphi_0(F)\,\mathrm{d}\mu_{x_p}\,\mathrm{d}x_p, \tag{14}$$

where $\mu \in L^\infty_w(\omega; \mathrm{rca}(\mathbb{R}^{3\times 2}))$. In addition, they have shown a certain uniqueness of the limiting stored energy density, i.e., that among all continuous integrands with p-th growth φ_0 is the sole function the Young-measure relaxation of which is equal to $\mathcal{I}_{\mathcal{FP}}$ for every linear boundary condition. More precisely, if denoting

$$W^{1,p}_A(\omega;\mathbb{R}^3) = \{w \in W^{1,p}(\omega;\mathbb{R}^3) \colon w(x) = Ax \text{ on } \gamma_0 \subset \partial\omega,\ \mathrm{meas}(\gamma_0) > 0\} \tag{15}$$

for a real matrix $A \in \mathbb{R}^{3\times 2}$ and let, on one hand, $Q[\mathcal{I}_\psi, A]$ be the relaxation, i.e., the lower-semicontinuous envelope, of

$$\mathcal{I}_\psi(y) = \int_\omega \psi(\nabla_p y)\,\mathrm{d}x_p, \tag{16}$$

where $\psi \colon \mathbb{R}^{3\times 2} \to \mathbb{R}$ is continuous with p-th growth, cf. (4) with $A \in \mathbb{R}^{3\times 2}$, on $W^{1,p}_A(\omega;\mathbb{R}^3)$ with respect to the weak topology, and $Y[\mathcal{I}_\psi, A]$ be the relaxation of

$$\mathcal{I}^*_\psi(\nu) = \begin{cases} \mathcal{I}_\psi(y) & \text{if } \nu = \delta_{\nabla_p y} \text{ for some } y \in W^{1,p}_A(\omega;\mathbb{R}^3), \\ +\infty & \text{otherwise in } L^\infty_w(\omega; \mathrm{rca}(\mathbb{R}^{3\times 2})) \end{cases} \tag{17}$$

with respect to the weak* topology of $L^\infty_w(\omega; \mathrm{rca}(\mathbb{R}^{3\times 2}))$. Then it can be shown that

$$\mathcal{I}_{\mathcal{LDR}}(y) = Q[\mathcal{I}_{\varphi_0}, A](y) \quad \text{and} \quad \mathcal{I}_{\mathcal{FP}}(\mu) = Y[\mathcal{I}_{\varphi_0}, A](\mu). \tag{18}$$

Furthermore, for all $A \in \mathbb{R}^{3\times 2}$ it holds that

$$Y[\mathcal{I}_\psi, A] = Y[\mathcal{I}_{\varphi_0}, A] \quad \Rightarrow \quad \psi \equiv \varphi_0. \tag{19}$$

cf. Freddi and Paroni (2004), Section 7 for more details. Note that an analogue does not hold in the case of $\mathcal{I}_{\mathcal{LDR}}$ as there are infinitely many functions with a quasiconvex envelope equal to $Q\varphi$.

Another approach was chosen by Bhattacharya and James (1999) who considered the total energy as the Helmholtz free energy augmented with an interfacial energy, a term penalizing the oscillations of the deformation gradient between different phases (as real materials do not develop inifinitely fine-scale lamination either), namely, $I_h(y)$ of the form

$$I_h(y) = \int_{\Omega_h} \varphi(\nabla y) + \kappa|\nabla^2 y|^2\,\mathrm{d}x, \tag{20}$$

where $\kappa > 0$ taken small but fixed. This additional term—yielding a smoothing effect—results in a limit energy density which needs no relaxation, an interfacial term still present, though, namely

$$\mathcal{I}_{\mathcal{BJ}}(y,b) = \int_\omega \varphi(y_{,1}|y_{,2}|b) + \kappa^2\{|\nabla_p^2 y|^2 + 2|\nabla_p b|^2\}\,\mathrm{d}x_p. \tag{21}$$

Note that the deformation of the thin film is described by two vector fields, $y\colon \omega \to \mathbb{R}^3$ holding the information about the mid-plane deformation of the film and $b\colon \omega \to \mathbb{R}^3$ outlining the behaviour of the cross-section of the film under loading.

One year later it was Shu (2000) who showed that if κ is also taken dependent on the material thickness $\kappa = \kappa(h)$ then the limit functional $\mathcal{I}_{\mathcal{LDR}}$ may be recovered for $h \to 0_+$ and $\kappa(h) \to 0_+$—independently of the ratio κ/h.

More recently, in order to derive rigorously a limiting thin film theory in the absence of an interfacial term while still recovering the aforementioned Cosserat vector field b Bocea (2007) introduced the scaled gradient Young measures, which are Young measures generated by sequences of scaled gradients of the form $\{(\nabla_p w_k \big| \frac{1}{h_k}\nabla_3 w_k)\}_{k\in\mathbb{N}}$, $h_n \to 0_+$.

When defining the set of all scaled gradient Young measures with underlying deformation $y \in W^{1,p}(\Omega;\mathbb{R}^3)$ and associated Cosserat vector $b \in L^p(\Omega;\mathbb{R}^3)$ as

$$\mathcal{G}^p_{y,b}(\Omega;\mathbb{R}^{3\times3}) := \Big\{\mu \in L^\infty_w(\Omega;\mathbb{R}^{3\times3}) \;\Big|\; \exists h_n \to 0_+ \; \exists\{y_n\} \subset W^{1,p}(\Omega;\mathbb{R}^3) : \\ y_n \rightharpoonup y, \quad \frac{1}{h_n}\nabla_3 y_n \rightharpoonup c, \quad \delta_{\left(\nabla_p y_n \big| \frac{1}{h_n}\nabla_3 y_n\right)} \overset{*}{\rightharpoonup} \mu\Big\}, \tag{22}$$

where the weak convergences are taken subsequently in the spaces $W^{1,p}(\Omega;\mathbb{R}^3)$, $L^p(\Omega;\mathbb{R}^3)$ and the dual space $L^\infty_w(\Omega;\mathrm{rca}(\mathbb{R}^{3\times3}))$, respectively, then the following assertion for the asymptotic limit holds:

$$\mathcal{I}_{\mathcal{B}}(y,b) = \min_{\mu\in\mathcal{G}^p_{y,c}(\Omega;\mathbb{R}^{3\times3})} \int_\Omega \varphi\,\mathrm{d}\mu. \tag{23}$$

This results from the decomposition of the sequence of scaled gradients into a p-equiintegrable part carrying the oscillations and a remainder accounting for the concentrations (but converging to zero in measure), cf. Bocea (2008); Bocea and Fonseca (2002); Braides and Zeppieri (2007). However, the set of scaled gradient Young measures still lacks any effective analytical description analogous to the one of gradient Young measures by Kinderlehrer and Pedregal (1994).

3.2 Compatibility Condition for the Deformation

In what follows, we will concentrate on the thin-film model proposed by Bhattacharya and James (1999) in order to implement it and make numerical simulations for a NiMnGa alloy.

For a deformation which does not tear the film apart, the Hadamard jump condition ought to be satisfied, which turns out to be essentially different from the bulk case. This condition requires in the thin film theory the existence of an invariant line interface between two (suitably rotated) zero-energy deformation gradients under a given deformation (the deformation gradient and the Cosserat vector may, however, suffer jumps across the interface). More precisely, let $\omega = \omega_1 \cup \omega_2 \cup \mathcal{L}$, where ω_1 and ω_2 are two disjoint subsets and $\mathcal{L}$ is a line segment between them. Then, if

$$(y_{,1}|y_{,2}|b) = \begin{cases} Q_1 U & \text{in } \omega_1 \\ Q_2 V & \text{in } \omega_2, \end{cases} \tag{24}$$

y denoting the deformation, b the associated Cosserat vector, while $U \neq V$ are two Bain matrices, Bhattacharya and James (1999) showed that the thin-film twinning equation may be expressed as

$$QU - V = a \otimes n + c \otimes e_3, \tag{25}$$

for suitable $Q \in SO(3)$, $a, n, c \in \mathbb{R}^3$ such that $n \cdot e_3 = 0$. Note that this condition is much weaker than the one required in 3D, i.e., rank$(QU - V) = 1$, which predicts the need of a planar interface between the energy wells. As a consequence, there might exist interfaces between particular phases in thin films which do not in the bulk material. E.g., there are certain materials which may exhibit a sharp interface between the austenite and the martensite, this phenomenon being theoretically impossible in the 3D setting.

4 Numerical Experiments

4.1 Sequential Laminates

Due to the non-local character of quasiconvexity it is difficult in most of the cases to compute the quasiconvex envelope of a particular function explicitly.

Therefore, one is pursuaded to consider a more general type of convexity, namely, the rank-one convexity which is defined as the property of a function $f\colon \mathbb{R}^{m\times m} \to \mathbb{R}$ being convex along rank-one connected matrices, i.e.,

$$f(\lambda A + (1-\lambda)B) \le \lambda f(A) + (1-\lambda)f(B) \quad \text{whenever} \quad \text{rank}(A-B) \le 1 \text{ and } 0 \le \lambda \le 1. \tag{26}$$

When introducing the rank-one convex envelope, analogously to the quasiconvex envelope, as

$$R\varphi = \sup\{\psi\colon \psi \le \varphi,\ \psi \text{ rank-one convex}\} \tag{27}$$

one can easily see that it provides an upper bound for the quasiconvex envelope

$$Q\varphi \le R\varphi \le \varphi. \tag{28}$$

A useful approximation procedure of this envelope is proposed by Kohn and Strang (1986), namely

Proposition 1. (see (Kohn and Strang, 1986, II)) Let $f\colon \mathbb{R}^{3\times 3} \to \mathbb{R}^3$ be bounded from below, then for every $A \in \mathbb{R}^{3\times 3}$ it holds that

$$Rf(A) = \lim_{k\to+\infty} R_k f(A), \tag{29}$$

where

$$R_0 f(A) = f(A), \tag{30}$$

then subsequently for $k = 1, 2, \dots$

$$R_k f(A) = \inf_{(\lambda, A_0, A_1)\in\mathcal{M}_A} \big(\lambda R_{k-1} f(A_0) + (1-\lambda) R_{k-1} f(A_1)\big), \tag{31}$$

$R_k f$ called k-th order laminate, and the set of admissible microstructures $\mathcal{M}_A \subset [0,1] \times \mathbb{R}^{3\times 3} \times \mathbb{R}^{3\times 3}$ for the matrix A defined as

$$\mathcal{M}_A = \{(\lambda, A_0, A_1)\colon A = \lambda A_0 + (1-\lambda)A_1 \text{ and } \text{rank}(A_1 - A_0) \le 1\}. \tag{32}$$

Hence, utilizing this latter characterization of rank-one convex envelope one can state the minimization problem for $k \in \mathbb{N}$ as

$$\begin{aligned} &\text{Minimize} \quad \mathcal{I}_{R_k}(y) = \int_\Omega R_k\varphi(\nabla y(x))\,\mathrm{d}x \\ &\text{subject to} \quad y \in \mathfrak{A}_{y_0}, \end{aligned} \tag{33}$$

and observe that

$$\min\,(6) = \inf\,(33) = \inf\,(1) \tag{34}$$

for all $k \in \mathbb{N}$, which follows from the inequality $Q\varphi \le R\varphi \le \cdots \le R_2\varphi \le R_1\varphi \le \varphi$ and relation (10).

In our simulations the first order laminate was used to approximate the rank-one convex envelope of the free energy density (21) while considering the contribution of the interfacial energy negligible, therefore setting the interfacial parameter $\kappa = 0$.

In order to set the numerical model let us first, by combining the thin-film twinning equation and the expression for the first order laminate, i.e.,

$$\begin{aligned}(y_{,1}|y_{,2}|b) &= \lambda A_0 + (1-\lambda)A_1,\\ A_1 - A_0 &= a\otimes n + c\otimes e_3,\end{aligned} \tag{35}$$

for some $a, n, c \in \mathbb{R}^3$ such that $n\cdot e_3 = 0$, express

$$\begin{aligned}A_0 &= (y_{,1}|y_{,2}|b) - (1-\lambda)(a\otimes n + c\otimes e_3),\\ A_1 &= (y_{,1}|y_{,2}|b) + \lambda(a\otimes n + c\otimes e_3).\end{aligned} \tag{36}$$

Furthermore, let us consider the finite element discretization, more precisely element-wise affine approximation for the deformation y and element-wise constant one for the other variables, by introducing

$$\begin{aligned}\mathcal{U}_d &\equiv \{v\in C(\bar\omega;\mathbb{R}^3)\colon v|_K \in P_0 \text{ for each } K\in\mathcal{T}_d,\ v = y_0 \text{ on } \Gamma\},\\ \mathcal{V}_d &\equiv \{v\colon \omega\to\mathbb{R}^3\colon v|_K\in P_0 \text{ for each } K\in\mathcal{T}_d\},\\ \mathcal{W}_d &\equiv \{v\colon \omega\to[0,1]\colon v|_K\in P_0 \text{ for each } K\in\mathcal{T}_d\},\end{aligned} \tag{37}$$

where $d > 0$ is the discretization parameter and $\mathcal{T}_d$ a triangulation of the reference domain ω.

Hence, the numerical minimization problem written in terms of the variables y, b, a, n, c and λ is

$$\begin{aligned}\text{Minimize}\quad & \mathcal{J}_{R_1}(y,b,a,n,c,\lambda)\\ \text{subject to}\quad & y\in\mathcal{U}_d,\\ & b,a,n,c\in\mathcal{V}_d,\\ & n\cdot e_3 = 0,\\ & \lambda\in\mathcal{W}_d,\end{aligned} \tag{38}$$

where the total free energy takes the form

$$\int_\omega \big\{\lambda\varphi((y_{,1}|y_{,2}|b) - (1-\lambda)(a\otimes n + c\otimes e_3)) + (1-\lambda)\varphi((y_{,1}|y_{,2}|b) + \lambda(a\otimes n + c\otimes e_3))\big\}\,\mathrm{d}x, \tag{39}$$

following from (31) for $k = 1$.

4.2 Tension and Compression Experiment for a Ni-Mn-Ga Single Crystal

Let us consider the Ni_2MnGa alloy and demonstrate using the numerical scheme described above the predicted austenite-martensite interface.

This alloy exhibits a cubic-to-tetragonal phase transformation with martensitic wells $U_1 = \text{diag}(\nu_1,\nu_2,\nu_2)$, $U_2 = \text{diag}(\nu_2,\nu_1,\nu_2)$, $U_3 = \text{diag}(\nu_2,\nu_2,\nu_1)$ for lattice parameters $\nu_1 = 1.13$, $\nu_2 = 0.9512$, and is modelled by a St. Venant–Kirchhoff type free energy density

$$\varphi(F) = \min_{i=0,\dots,3}\varphi_i(F) = \min_{i=0,\dots,3}\frac{1}{2}(F-U_i)\cdot\mathbb{C}^i(F-U_i) \tag{40}$$

for all $F\in\mathbb{R}^{3\times3}$, where the tensors of elastic moduli $\mathbb{C}^i$ take—using the Voigt notation—the values $\mathbb{C}^0_{11} = 13.6$ GPa, $\mathbb{C}^0_{12} = 9.2$ GPa, $\mathbb{C}^0_{44} = 10.2$ GPa for the austenite and $\mathbb{C}^i_{11} = 136$ GPa, $\mathbb{C}^i_{12} = 92$ GPa, $\mathbb{C}^i_{44} = 102$ GPa, $i = 1,2,3$, equally for all martensitic variants, inspired by the work of Kružík and Roubíček (2004).

In both the tension and compression experiments as reference configuration $\omega = (0,9)\times(0,4)$ is taken in the stress-free austenitic phase, cf. Figure 2 prescribing zero displacement Dirichlet boundary condition on Γ_{id}. On Γ_{pre} we have prescribed a given elongation.

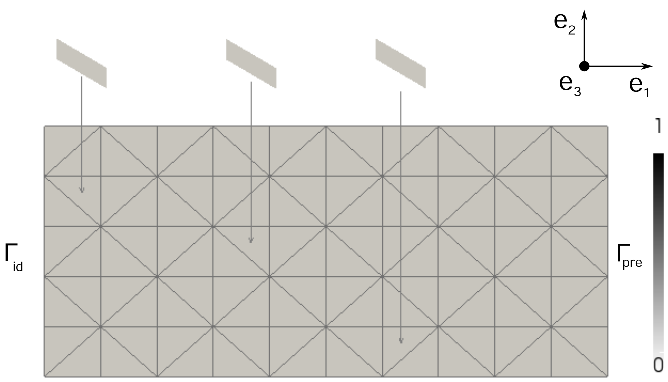

Figure 2: Reference configuration of Ni_2MnGa single crystal thin film in stress-free austenite (white)—Γ_{id} fixed boundary segment, Γ_{pre} boundary segment with prescribed elongation

The first-order laminate is, however, capable only of capturing two phase variants, therefore we had to select the competing wells with the greatest impact on the behaviour of the specimen, in our cases these were the austenite U_0 and the martensitic variant $U_1 = \text{diag}(\nu_1, \nu_2, \nu_2)$, resp. $U_2 = \text{diag}(\nu_2, \nu_1, \nu_2)$ for the tension, resp. compression test.

The minimization procedure has been done with the aid of the limited memory L-BFGS-B routine—developed by Byrd et al. (1995)—which is, however, designed for local optimization. Therefore, a successful computation of our global minimization problem, being, moreover, non-convex, is a challanging task which requires a good initial guess of the variables—involving the explicit computation of the interface between compatible wells. Afterwards, the visualization of the different fractions of the martensitic variants was completed by evaluating

$$\gamma(K) = \sum_{l=0}^{1} \lambda_l \frac{|(A_l^K)^T A_l^K - U_i^T U_i|^2}{|(A_l^K)^T A_l^K - U_0^T U_0|^2 + |(A_l^K)^T A_l^K - U_i^T U_i|^2} \tag{41}$$

on each element K of the triangulation with $\lambda_0 = \lambda$ and $\lambda_1 = 1 - \lambda$, then interpolating on the black–white scale as seen on Figure 3 and Figure 4 (the austenite is coloured white, the martensite black).

Note that as a result of the simplied model we used, the first-order laminate and the method of prescribing the elongation on Γ_{pre}, the elements at the fixed boundary parts cannot undergo phase transformation. Therefore Figure 3 exhibits certain unnatural symmetries in the volume fraction of the martensite—the austenite–martensite transformation is known to start in a corner of the specimen. However, our simulation was able to recover the nonlinear response of the material, specific for SMAs, under strain, cf. the stess–strain plot in Figure 3.

The compression experiment in Figure 4 shows a specific feature of thin films not observed in the bulk. When compressed, under a small back pressure, they bulge up without changing phase, i.e., the material persists in the austenite. This buckling effect has been proposed in Bhattacharya and James (1999), here simulated explicitly, and predicts that some theoretical tools, e.g., the non-buckling-type assumption (3.18) in Mielke and Roubíček (2003), might be natural in the bulk, but are never in the thin-film theory and should be avoided.

Another specific type of buckling related to the microactuation character of shape-memory alloys has been numerically investigated by Dondl et al. (2007).

5 Conclusion

The aim of this contribution was to draw attention to the difference between the modelling of bulk and thin film shape-memory materials with particular stress on richer structure of interfaces in some alloys, which first appeared in Bhattacharya and James (1999).

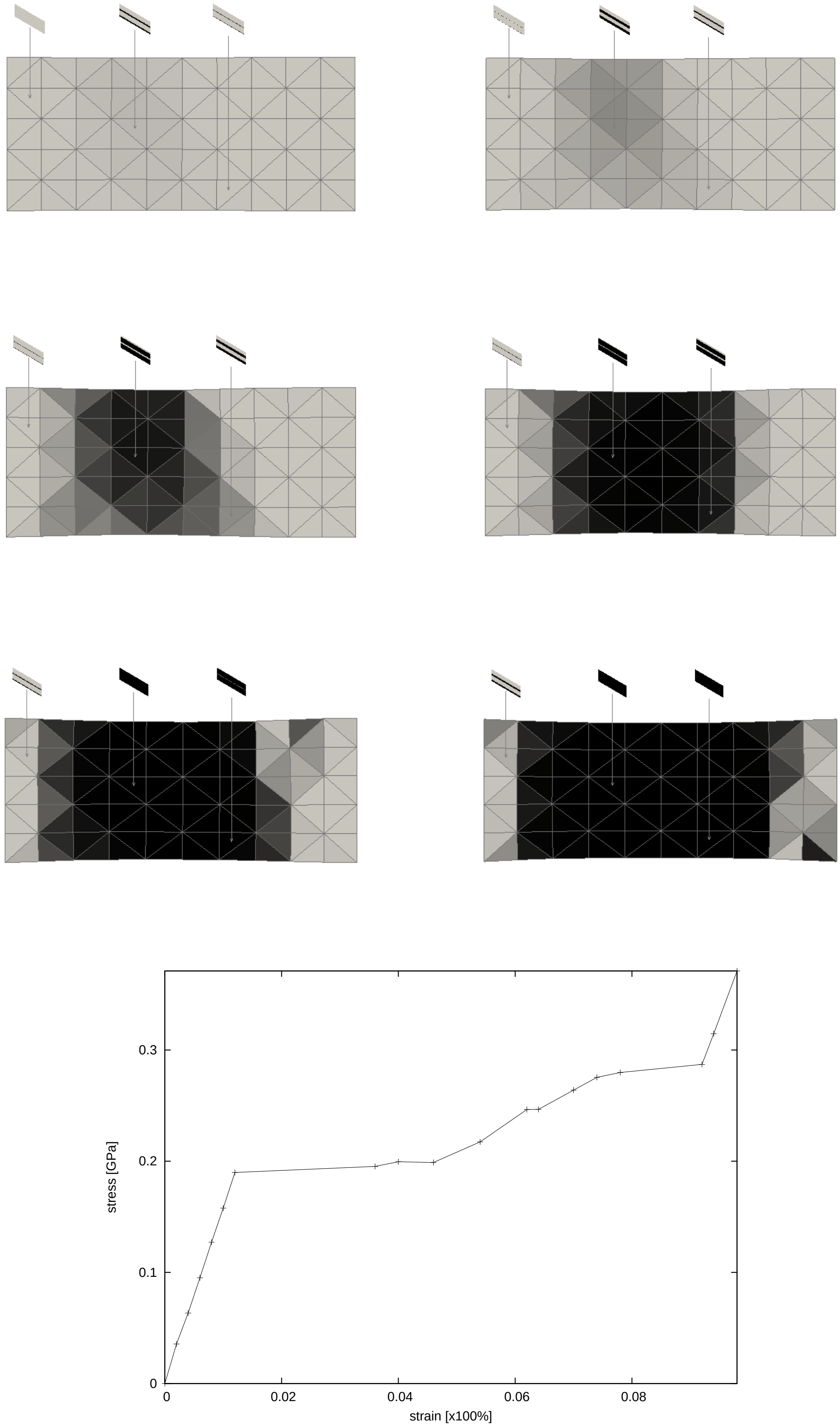

Figure 3: Tension experiment for Ni_2MnGa single crystal with 1, 2, 4, 6, 8 and 10% elongation in the x-direction and its stress–strain curve

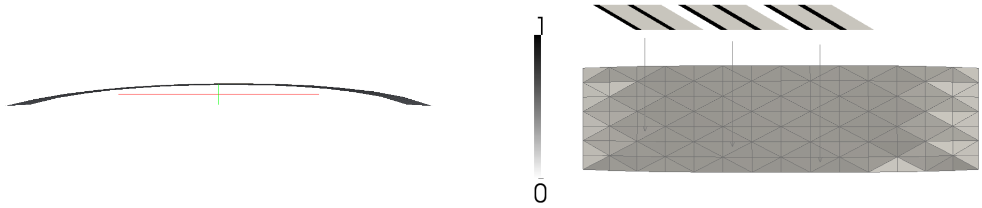

Figure 4: Side and top view on a 2% compressed Ni_2MnGa single crystal sheet with small back pressure exhibiting buckling with negligible phase transformation

To this behalf, after a brief overview of the different approaches to the derivation of a 2D model we have done some simple numerical calculations on an academic SMA alloy to justify the theoretical tools introduced.

As already pointed out before, a gradient-based optimization algorithm is not the most effective way to treat the non-convex minimization problem related to SMAs which usually possesses many local minima. Another interesting concept is to adopt a global optimization routine, e.g., particle swarm optimization (PSO), cf. Benešová (2011) for some promising results in 3D. However, these metaheuristic algorithms, such as the PSO and other genetic algorithms, do not guarantee that an optimal solution is ever found at all. Cf. Yang (2008) for an extensive overview of the topic.

Other future work will focus on the evolutionary problems in the thin film theory of shape-memory alloys which lacks an effective description till nowadays, the numerical method described above could then be easily extended to the dissipative evolutionary model.

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Chapter 4

Young measures supported on invertible matrices

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Young measures supported on invertible matrices

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Motivated by variational problems in non-linear elasticity, we explicitly characterize the set of Young measures generated by gradients of a uniformly bounded sequence in $W^{1,\infty}(\Omega;\mathbb{R}^n)$ where the inverted gradients are also bounded in $L^\infty(\Omega;\mathbb{R}^{n\times n})$. This extends the original results due to the studies of Kinderlehrer and Pedregal. Besides, we completely describe Young measures generated by a sequence of matrix-valued mappings $\{Y_k\}_{k\in\mathbb{N}} \subset L^p(\Omega;\mathbb{R}^{n\times n})$, such that $\{Y_k^{-1}\}_{k\in\mathbb{N}} \subset L^p(\Omega;\mathbb{R}^{n\times n})$ is bounded, too, and the generating sequence satisfies the constraint $\det Y_k > 0$.

Keywords: orientation-preserving mappings; relaxation; Young measures

AMS Subject Classifications: 49J45; 35B05

1. Introduction

In this paper, we investigate a new tool to study minimization problems for integral functionals defined over matrix-valued mappings that take values only in the set of invertible matrices. Typical examples are found, e.g. in non-linear elasticity where static equilibria are minimizers of the elastic energy

$$J(y) := \int_\Omega W(\nabla y(x))\,\mathrm{d}x, \tag{1.1}$$

where $\Omega \subset \mathbb{R}^n$ denotes the reference configuration of the material, $y \in W^{1,p}(\Omega;\mathbb{R}^n)$ is the deformation, $1 < p \le +\infty$, $y = y_0$ on $\partial\Omega$ and $W\colon \mathbb{R}^{n\times n} \to \mathbb{R}$ is the stored energy density, i.e. the potential of the first Piola–Kirchhoff stress tensor. Further, usually in elasticity, one demands either $\det \nabla y \neq 0$ to assure local invertibility of ∇y or even $\det \nabla y > 0$ in order to preserve orientation of y.

If W is polyconvex, i.e. $A \mapsto W(A)$ can be written as a convex function of all minors of A, then the existence of minimizers to (1.1) was proved by J.M. Ball in his pioneering

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paper [1]. We refer, for example, to [2,3] for various further results in this direction. Namely, the existence theory for polyconvex materials can even cope with the important physical assumption

$$W(A) \to +\infty \text{whenever } \det A \to 0_+. \tag{1.2}$$

On the other hand, there are many materials that cannot be modelled by polyconvex stored energies, prominent examples are materials with microstructure, like shape-memory materials [4,5]. If we give up (1.2) and suppose that W has polynomial growth at infinity, i.e. there exist $c, \tilde{c} > 0$ such that

$$c(-1 + |A|^p) \leq W(A) \leq \tilde{c}(1 + |A|^p), \tag{1.3}$$

the existence of a solution to (1.1) is guaranteed if W is quasiconvex [6], which means that for all $\varphi \in W_0^{1,\infty}(\Omega; \mathbb{R}^n)$ and all $A \in \mathbb{R}^{n\times n}$ it holds that

$$|\Omega| W(A) \leq \int_\Omega W(A + \nabla\varphi(x))\, \mathrm{d}x. \tag{1.4}$$

However, stored energy densities of materials with microstructure do not possess this property either. As a result, solutions to (1.1) might not exist. Various relaxation techniques were developed [3,5,7] and used in numerical approximations [8] to overcome this drawback for integrands satisfying (1.3). Some relaxation results for the case $W(A) \to +\infty$ if $\det A \to 0$ but $W(A) < +\infty$ even if $\det A < 0$ were recently stated in [9]. In both situations, one replaces the integrand by its quasiconvex envelope (the pointwise supremum of all quasiconvex functions not greater than W).

Another approach is to extend the notion of solutions from Sobolev mappings to parameterized measures called Young measures [7,10–14,30]. The idea is to describe the limit behaviour of $\{J(y_k)\}_{k\in\mathbb{N}}$ along a minimizing sequence $\{y_k\}_{k\in\mathbb{N}}$. Nevertheless, the growth condition (1.3) is still a key ingredient in these considerations.

Our goal is to tailor the Young-measure relaxation to functions satisfying (1.2). In order to reach this, we allow W to depend on the inverse of its argument, more precisely, we suppose that W is continuous on invertible matrices and that there exist positive constants $c, \tilde{c} > 0$ such that

$$c(-1 + |A|^p + |A^{-1}|^p) \leq W(A) \leq \tilde{c}(1 + |A|^p + |A^{-1}|^p). \tag{1.5}$$

Notice that (1.5) implies (1.2) and that W has polynomial growth in $|A|$ and $|A^{-1}|$ at infinity. In the context of non-linear elasticity, A plays the role of a deformation gradient measuring deformation strain and A^{-1} is just another strain measure. We refer, for example e.g. to [15,16] for the so-called Seth–Hill family of strain measures or to [17] where the physical meaning of the Piola tensor and of the Finger tensor depending on $A^{-1}A^{-\top}$ and on $A^{-\top}A^{-1}$, respectively, is discussed in great detail.

To justify (1.5), we notice that if $y : \Omega \to \mathbb{R}^n$ is a deformation of the reference domain $\Omega \subset \mathbb{R}^n$ and $y^{-1} : y(\Omega) \to \Omega$ is its differentiable inverse then, for $x \in \Omega$ $(\nabla y(x))^{-1} = \nabla y^{-1}(z)$, $z := y(x)$. Hence, if we exchange the role of the reference and deformed configurations, our model requires the same integrability for the original deformation gradient as well as for the deformation gradient of the inverse deformation. Also, if we consider $n = 3$, $p \geq 2$, $q \geq 1$ satisfying $r := pq/(p + 2q) \geq 1$, and a polyconvex stored energy density of the form

$$W(F) := \begin{cases} |F|^p + 1/(\det F)^q & \text{if } \det F > 0 \\ +\infty \text{ otherwise} \end{cases}$$

then we see that every minimizing sequence $\{y_k\}_{k\in\mathbb{N}} \subset W^{1,p}(\Omega;\mathbb{R}^n)$ of J from (1.1) is such that $\{\|(\nabla y_k)^{-1}\|_{L^r(\Omega;\mathbb{R}^{n\times n})}\}_{k\in\mathbb{N}}$ is bounded by a constant independent of $k \in \mathbb{N}$. Hence, boundedness of the sequences of "inverted gradients" $\{(\nabla y_k)^{-1}\}_{k\in\mathbb{N}}$ in some Lebesgue space may appear as a necessary condition on minimizing sequences in non-linear elasticity. On the other hand, if W satisfies (1.5) then $\{1/\det\nabla y_k\}_{k\in\mathbb{N}}$ is bounded in $L^p(\Omega)$ for any minimizing sequence $\{y_k\}_{k\in\mathbb{N}}$ of J.

This all motivates the idea to perform relaxation in terms of gradient Young measures generated by gradients of functions $\{y_k\}_{k\in\mathbb{N}} \subset W^{1,p}(\Omega;\mathbb{R}^n)$ such that $\{(\nabla y_k)^{-1}\}_{k\in\mathbb{N}} \subset L^p(\Omega;\mathbb{R}^{n\times n})$ is bounded, too. In order to do so, an explicit characterization of this specific set of measures is essential. In this work, however, we concentrate merely on parameterized measures generated by gradients of Lipschitz maps. Therefore, these results should be understood as a first step in the analysis of more realistic hyperelastic models where p is finite.

In particular, we completely and explicitly describe Young measures generated by gradients of functions $\{y_k\}_{k\in\mathbb{N}} \subset W^{1,\infty}(\Omega;\mathbb{R}^n)$ with $\{(\nabla y_k)^{-1}\}_{k\in\mathbb{N}} \subset L^\infty(\Omega;\mathbb{R}^{n\times n})$ also bounded. The main characterization is exposed in Theorem 2.5 following the work [18], only additional constraints on the support of the measure and a restricted set of test functions for the Jensen inequality needs to be introduced for which the envelope from (1.10) does not need to be quasiconvex anymore.

Moreover, we also characterize Young measures generated by matrix-valued mappings $\{Y_k\}_{k\in\mathbb{N}} \subset L^p(\Omega;\mathbb{R}^{n\times n})$ with $\{Y_k^{-1}\}_{k\in\mathbb{N}} \subset L^p(\Omega;\mathbb{R}^{n\times n})$ bounded. Namely, we show that, in this case, the Young measures are necessarily supported on invertible matrices and satisfy a certain integral condition, cf. (2.1), Theorem 2.2 and Proposition 2.4. Contrary to the general theory of Young measures generated by L^p-maps [7,19], where only the behaviour of test functions at infinity is important, Young measures supported on invertible matrices are also sensitive to the asymptotics of test functions as the argument approaches a singular matrix. The constraint $\det Y_k > 0$ almost everywhere in Ω can be incorporated, too.

Let us mention that while the matrix case is an extension of the results due to Freddi and Paroni [20] who considered a related case for vector-valued maps, the results concerning the curl constraint are the main novelty of the paper. We refer also to [21] for another refinement of Young measures involving discontinuous integrands.

The plan of the paper is as follows. After introducing Young measures we state our main results – Theorems 2.1, 2.2 and 2.5 in Section 2. The proofs of our statements are left, however, to Section 3 for the L^p-case and Section 4 for the $W^{1,\infty}$-case. In particular, Propositions 3.1 and 3.2 are of special interest as they form an L^∞-version of our main Theorems 2.1 and 2.2.

1.1. *Notation*

Throughout the paper, we use standard notation for Lebesgue L^p, Sobolev $W^{1,p}$ spaces and the space $C(S)$ of continuous functions on $S \subset \mathbb{R}^n$. If not said otherwise, $\Omega \subset \mathbb{R}^n$ is a bounded domain with Lipschitz boundary. For $p \geq 0$, we define the following subspace of $C(\mathbb{R}^{n\times n})$:

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

$\mathbb{R}^{n\times n}_{\mathrm{inv}}$ shall denote the set of invertible matrices in $\mathbb{R}^{n\times n}$ and $\mathbb{R}^{n\times n}_{\mathrm{inv}+}$ denotes the set of matrices in $\mathbb{R}^{n\times n}$ with positive determinant. Further, we define the following subsets of the set of invertible matrices:

$$R^{n\times n}_{\varrho} := \{A \in \mathbb{R}^{n\times n}_{\mathrm{inv}};\ \max(|A|, |A^{-1}|) \leq \varrho\}, \tag{1.6}$$

$$R^{n\times n}_{\varrho+} := \{A \in R^{n\times n}_{\varrho};\ \det A > 0\} \tag{1.7}$$

for $0 < \varrho < \infty$, while $R^{n\times n}_{+\infty} := \mathbb{R}^{n\times n}_{\mathrm{inv}}$. Note that both $R^{n\times n}_{\varrho}$ and $R^{n\times n}_{\varrho+}$ are compact for every $1 \leq \varrho < \infty$ and empty for $\varrho < 1$.

When analysing the $W^{1,\infty}$-case, we shall need, for $\varrho \in [1; +\infty]$, the following set

$$\mathcal{O}(\varrho) := \{v : \mathbb{R}^{n\times n} \to \mathbb{R} \cup \{+\infty\};\ v \in C(R^{n\times n}_{\varrho}),\ v(s) = +\infty \text{ if } s \in \mathbb{R}^{n\times n} \setminus R^{n\times n}_{\varrho}\}. \tag{1.8}$$

In the L^p-case, we will work with the following subspace of $C(\mathbb{R}^{n\times n}_{\mathrm{inv}})$

$$C_{p,-p}(\mathbb{R}^{n\times n}_{\mathrm{inv}}) := \left\{ v \in C(\mathbb{R}^{n\times n}_{\mathrm{inv}});\ \lim_{|s|+|s^{-1}|\to\infty} \frac{v(s)}{|s|^p + |s^{-1}|^p} = 0 \right\} \tag{1.9}$$

and $C^{p,-p}(\mathbb{R}^{n\times n}_{\mathrm{inv}})$ is defined as

$$C^{p,-p}(\mathbb{R}^{n\times n}_{\mathrm{inv}}) := \{f \in C(\mathbb{R}^{n\times n}_{\mathrm{inv}});\ |f(s)| \leq C(1 + |s|^p + |s^{-1}|^p)\ \forall s \in \mathbb{R}^{n\times n}_{\mathrm{inv}}\};$$

here and in the sequel $|A|$ is the spectral norm of the matrix A, i.e. the largest singular value of A (the largest eigenvalue of $\sqrt{AA^{\mathrm{T}}}$).

If $v : \mathbb{R}^{n\times n} \to \mathbb{R} \cup \{+\infty\}$ is bounded from below and Borel measurable we define

$$Z^{\infty}v(A) := \inf_{\varphi \in W^{1,\infty}_A(\Omega;\mathbb{R}^n)} |\Omega|^{-1} \int_{\Omega} v(\nabla\varphi(x))\,\mathrm{d}x, \tag{1.10}$$

where $W^{1,\infty}_A(\Omega; \mathbb{R}^n) := \{\psi \in W^{1,\infty}(\Omega; \mathbb{R}^n);\ \psi(x) = Ax \text{ for } x \in \partial\Omega\}$.

It is well known that the right-hand side of (1.10) is the same if we replace Ω by any other bounded Lipschitz domain in $\mathbb{R}^n$.

Note that v is quasiconvex if $v = Z^{\infty}v$. The quasiconvex envelope of v, Qv is defined as:

$$Qv(A) := \sup\{g(A);\ g : \mathbb{R}^{n\times n} \to \mathbb{R} \cup \{+\infty\};\ g \leq v,\ g \text{ is quasiconvex}\}.$$

We say that $\{u_k\}_{k\in\mathbb{N}} \subset L^1(\Omega)$ is equi-integrable if we can extract a subsequence weakly converging in $L^1(\Omega)$. We refer, e.g. to [11,22] for details about equi-integrability and relative weak compactness in $L^1(\Omega)$. Finally, C denotes a generic positive constant which may change from place to place.

1.2. *Young measures*

Young measures on a bounded domain $\Omega \subset \mathbb{R}^n$ are weakly* measurable mappings $x \mapsto \nu_x : \Omega \to \mathrm{rca}(\mathbb{R}^{n\times n})$ with values in probability measures; and the adjective "weakly* measurable" means that, for any $v \in C_0(\mathbb{R}^{n\times n})$, the mapping $\Omega \to \mathbb{R} : x \mapsto \langle \nu_x, v\rangle = \int_{\mathbb{R}^{n\times n}} v(s)\nu_x(\mathrm{d}s)$ is measurable in the usual sense. Let us remind that, by the Riesz theorem, $\mathrm{rca}(\mathbb{R}^{n\times n})$, normed by the total variation, is a Banach space which is isometrically isomorphic with $C_0(\mathbb{R}^{n\times n})^*$, where $C_0(\mathbb{R}^{n\times n})$ stands for the space of all continuous functions $\mathbb{R}^{n\times n} \to \mathbb{R}$ vanishing at infinity. Let us denote the set of all Young measures by $\mathcal{Y}(\Omega; \mathbb{R}^{n\times n})$. It is known that $\mathcal{Y}(\Omega; \mathbb{R}^{n\times n})$ is a convex subset of $L^\infty_{\mathrm{w}}(\Omega; \mathrm{rca}(\mathbb{R}^{n\times n})) \cong L^1(\Omega; C_0(\mathbb{R}^{n\times n}))^*$, where the subscript "w" indicates the aforementioned property of weak* measurability. Let $S \subset \mathbb{R}^{n\times n}$ be a compact set. A classical result [12,23] is that for every sequence $\{Y_k\}_{k\in\mathbb{N}}$ bounded in $L^\infty(\Omega; \mathbb{R}^{n\times n})$ such that $Y_k(x) \in S$, there exists a subsequence (denoted by the same indices for notational simplicity) and a Young measure $\nu = \{\nu_x\}_{x\in\Omega} \in \mathcal{Y}(\Omega; \mathbb{R}^{n\times n})$ satisfying

$$\forall v \in C(S) : \lim_{k\to\infty} v(Y_k) = \int_{\mathbb{R}^{n\times n}} v(s)\nu_x(\mathrm{d}s) \text{ weakly* in } L^\infty(\Omega). \tag{1.11}$$

Moreover, ν_x is supported on S for almost all $x \in \Omega$. On the other hand, if $\mu = \{\mu_x\}_{x\in\Omega}$, μ_x is supported on S for almost all $x \in \Omega$ and $x \mapsto \mu_x$ is weakly* measurable, then there exists a sequence $\{Z_k\}_{k\in\mathbb{N}} \subset L^\infty(\Omega; \mathbb{R}^{n\times n})$, $Z_k(x) \in S$ and (1.11) holds with μ and Z_k instead of ν and Y_k, respectively.

Let us denote by $\mathcal{Y}^\infty(\Omega; \mathbb{R}^{n\times n})$ the set of all Young measures that are created in this way, i.e. by taking all bounded sequences in $L^\infty(\Omega; \mathbb{R}^{n\times n})$. Moreover, we denote by $\mathcal{GY}^\infty(\Omega; \mathbb{R}^{n\times n})$ the subset of $\mathcal{Y}^\infty(\Omega; \mathbb{R}^{n\times n})$ consisting of measures generated by gradients of $\{y_k\}_{k\in\mathbb{N}} \subset W^{1,\infty}(\Omega; \mathbb{R}^n)$, i.e. $Y_k := \nabla y_k$ in (1.11). It is due to Kinderlehrer and Pedregal [18] that $\nu \in \mathcal{Y}^\infty(\Omega; \mathbb{R}^{n\times n})$ is in $\mathcal{GY}^\infty(\Omega; \mathbb{R}^{n\times n})$ if and only if

(1) there exists $z \in W^{1,\infty}(\Omega; \mathbb{R}^n)$ such that $\nabla z(x) = \int_{\mathbb{R}^{n\times n}} A\nu_x(\mathrm{d}A)$ for a.e. $x \in \Omega$,
(2) $\psi(\nabla z(x)) \le \int_{\mathbb{R}^{n\times n}} \psi(A)\nu_x(\mathrm{d}A)$ for a.e. $x \in \Omega$ and for all ψ quasiconvex, continuous and bounded from below,
(3) $\mathrm{supp}\, \nu_x \subset K$ for some compact set $K \subset \mathbb{R}^{n\times n}$ for a.e. $x \in \Omega$.

A generalization of the L^∞-result (1.11) was formulated by Schonbek [19] (cf. also [10]): if $1 \le p < +\infty$ then for every sequence $\{Y_k\}_{k\in\mathbb{N}}$ bounded in $L^p(\Omega; \mathbb{R}^{n\times n})$ there exists a subsequence (denoted by the same indices) and a Young measure $\nu = \{\nu_x\}_{x\in\Omega} \in \mathcal{Y}(\Omega; \mathbb{R}^{n\times n})$ such that

$$\forall v \in C_p(\mathbb{R}^{n\times n}) : \lim_{k\to\infty} v(Y_k) = \int_{\mathbb{R}^{n\times n}} v(s)\nu_x(\mathrm{d}s) \text{ weakly in } L^1(\Omega)\,. \tag{1.12}$$

We say that $\{Y_k\}_{k\in\mathbb{N}}$ generates ν if (1.12) holds. Let us denote by $\mathcal{Y}^p(\Omega; \mathbb{R}^{n\times n})$ the set of all Young measures that are obtained through the latter procedure, i.e. by taking all bounded sequences in $L^p(\Omega; \mathbb{R}^{n\times n})$. It was shown in [24] that if $\nu \in \mathcal{Y}(\Omega; \mathbb{R}^{n\times n})$ satisfies the bound

$$\int_\Omega \int_{\mathbb{R}^{n\times n}} |s|^p \nu_x(\mathrm{d}s)\, \mathrm{d}x < +\infty \tag{1.13}$$

then $\nu \in \mathcal{Y}^p(\Omega; \mathbb{R}^{n\times n})$.

2. Main results

Let us, at this point, summarize the main results of the paper.

2.1. L^p-case

We define the following subsets of $\mathcal{Y}^p(\Omega; \mathbb{R}^{n\times n})$:

$$\mathcal{Y}^{p,-p}(\Omega; \mathbb{R}^{n\times n}) := \Big\{\nu \in \mathcal{Y}^p(\Omega; \mathbb{R}^{n\times n});\ \int_\Omega \int_{\mathbb{R}^{n\times n}_{\rm inv}} (|s|^p + |s^{-1}|^p)\nu_x(\mathrm{d}s)\,\mathrm{d}x < +\infty,$$
$$\nu_x(\mathbb{R}^{n\times n}_{\rm inv}) = 1 \text{ for a.a. } x \in \Omega\Big\}, \tag{2.1}$$

$$\mathcal{Y}^{p,-p}_+(\Omega; \mathbb{R}^{n\times n}) := \left\{\nu \in \mathcal{Y}^{p,-p}(\Omega; \mathbb{R}^{n\times n});\ \nu_x(\mathbb{R}^{n\times n}_{\rm inv+}) = 1 \text{ for a.a. } x \in \Omega\right\}. \tag{2.2}$$

Our results concerning the L^p-case are then summarized in the following theorems.

THEOREM 2.1 *Let $+\infty > p \geq 1$, let $\Omega \subset \mathbb{R}^n$ be open and bounded, and let $\{Y_k\}_{k\in\mathbb{N}}$, $\{Y_k^{-1}\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{n\times n})$ be bounded. Then there is a subsequence of $\{Y_k\}_{k\in\mathbb{N}}$ (not relabelled) and $\nu \in \mathcal{Y}^{p,-p}(\Omega; \mathbb{R}^{n\times n})$ such that for every $g \in L^\infty(\Omega)$ and every $v \in C_{p,-p}(\mathbb{R}^{n\times n}_{\rm inv})$ it holds that*

$$\lim_{k\to\infty} \int_\Omega v(Y_k(x))g(x)\,\mathrm{d}x = \int_\Omega \int_{\mathbb{R}^{n\times n}_{\rm inv}} v(s)\nu_x(\mathrm{d}s)g(x)\,\mathrm{d}x, \tag{2.3}$$

Conversely, if $\nu \in \mathcal{Y}^{p,-p}(\Omega; \mathbb{R}^{n\times n})$ then there is a bounded sequence $\{Y_k\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{n\times n})$ such that $\{Y_k^{-1}\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{n\times n})$ is also bounded and (2.3) *holds for all g and v defined above.*

THEOREM 2.2 *Let $+\infty > p \geq 1$, let $\Omega \subset \mathbb{R}^n$ be open and bounded, and let $\{Y_k\}_{k\in\mathbb{N}}$, $\{Y_k^{-1}\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{n\times n})$ be bounded and for every $k \in \mathbb{N}$* $\det Y_k > 0$ *almost everywhere in Ω. Then there is a subsequence of $\{Y_k\}_{k\in\mathbb{N}}$ (not relabelled) and $\nu \in \mathcal{Y}^{p,-p}_+(\Omega; \mathbb{R}^{n\times n})$ such that for every $g \in L^\infty(\Omega)$ and every $v \in C_{p,-p}(\mathbb{R}^{n\times n}_{\rm inv})$* (2.3) *holds.*

Conversely, if $\nu \in \mathcal{Y}^{p,-p}_+(\Omega; \mathbb{R}^{n\times n})$ then there is a bounded sequence $\{Y_k\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{n\times n})$ such that $\{Y_k^{-1}\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{n\times n})$ is also bounded, for every $k \in \mathbb{N}$ $\det Y_k > 0$ *almost everywhere in Ω, and* (2.3) *holds for all g and v defined above.*

Remark 2.3 We could also define the sets

$$\mathcal{Y}^{p,f(\cdot)}(\Omega; \mathbb{R}^{n\times n}) := \Big\{\nu \in \mathcal{Y}^p(\Omega; \mathbb{R}^{n\times n});\ \int_\Omega \int_{\mathbb{R}^{n\times n}_{\rm inv}} (|s|^p + f(s^{-1}))\nu_x(\mathrm{d}s)\,\mathrm{d}x < +\infty\,,$$
$$\nu_x(\mathbb{R}^{n\times n}_{\rm inv}) = 1 \text{ for a.a. } x \in \Omega\Big\}, \tag{2.4}$$

$$\mathcal{Y}^{p,f(\cdot)}_+(\Omega; \mathbb{R}^{n\times n}) := \Big\{\nu \in \mathcal{Y}^p(\Omega; \mathbb{R}^{n\times n});\ \int_\Omega \int_{\mathbb{R}^{n\times n}_{\rm inv+}} (|s|^p + f(s^{-1}))\nu_x(\mathrm{d}s)\,\mathrm{d}x < +\infty\,,$$
$$\nu_x(\mathbb{R}^{n\times n}_{\rm inv+}) = 1 \text{ for a.a. } x \in \Omega\Big\}, \tag{2.5}$$

with $f(\cdot) \geq |\det(\cdot)|^q$ for some $q > 0$. Obvious modifications of the proofs below give that ν is in $\mathcal{Y}^{p,f(\cdot)}(\Omega; \mathbb{R}^{n\times n})(\mathcal{Y}^{p,f(\cdot)}_+(\Omega; \mathbb{R}^{n\times n}))$ if and only if it can be generated by a sequence of invertible matrices with inverses $\left\{Y_k^{-1}\right\}_{k\in\mathbb{N}}$ bounded in $L^q(\Omega; \mathbb{R}^{n\times n})$ (and $\det Y_k(x) > 0$ for all $k \in \mathbb{N}$ and a.a. $x \in \Omega$). Defining these sets allows us to relax even a larger class of functions than $C_{p,-p}(\mathbb{R}^{n\times n}_{\rm inv})$.

The next result shows that the weak limit of a sequence of gradients with positive determinant inherits this property if we control the behaviour of the inverse.

PROPOSITION 2.4 *Let $p > n$. If $y_k \rightharpoonup y$ in $W^{1,p}(\Omega;\mathbb{R}^n)$ is such that* $\det \nabla y_k > 0$ *a.e. in Ω for all $k \in \mathbb{N}$ and $\{(\nabla y_k)^{-1}\}_{k\in\mathbb{N}} \subset L^p(\Omega;\mathbb{R}^{n\times n})$ is bounded then* $\det \nabla y > 0$ *a.e. in Ω. Moreover, every Young measure generated by a subsequence of $\{\nabla y_k\}_{k\in\mathbb{N}}$ is supported on $\mathbb{R}^{n\times n}_{\mathrm{inv}+}$.*

2.2. $W^{1,\infty}$-case

We now turn to a characterization of gradient Young measures supported on invertible matrices. We shall see that the characterization is similar to the one obtained by Kinderlehrer and Pedregal for gradient Young measures [18,25], however, the set of test functions for the Jensen inequality is restricted to $\mathcal{O}(\varrho)$ from (1.8), it is not known if $Z^\infty v$ is still quasiconvex in this case.

Let us define the following sets of Young measures generated by bounded and invertible gradients of $W^{1,\infty}(\Omega;\mathbb{R}^n)$ maps:

$$\mathcal{GY}^{+\infty,-\infty}_\varrho(\Omega;\mathbb{R}^{n\times n}) := \Big\{\nu \in \mathcal{Y}^\infty(\Omega;\mathbb{R}^{n\times n});\ \exists\{y_k\}_{k\in\mathbb{N}} \subset W^{1,\infty}(\Omega;\mathbb{R}^n)\,, \\ \text{for a.a. } x\in\Omega\ \{\nabla y_k(x)\}_{k\in\mathbb{N}} \subset R^{n\times n}_\varrho \text{ and } \{\nabla y_k\}_{k\in\mathbb{N}} \text{ generates } \nu\Big\} \tag{2.6}$$

and $\mathcal{GY}^{+\infty,-\infty}(\Omega;\mathbb{R}^{n\times n}) := \bigcup_{\varrho>0}\mathcal{GY}^{+\infty,-\infty}_\varrho(\Omega;\mathbb{R}^{n\times n})$.

THEOREM 2.5 *Let $\nu \in \mathcal{Y}^\infty(\Omega;\mathbb{R}^{n\times n})$. Then $\nu \in \mathcal{GY}^{+\infty,-\infty}(\Omega;\mathbb{R}^{n\times n})$ if and only if the following three conditions hold:*

$$\operatorname{supp}\nu_x \subset R^{n\times n}_\varrho \textit{ for a.a. } x\in\Omega \textit{ and some } \varrho\ge 1, \tag{2.7}$$

$$\exists\, u \in W^{1,\infty}(\Omega;\mathbb{R}^n)\ :\ \nabla u(x) = \int_{\mathbb{R}^{n\times n}_{\mathrm{inv}}} s\nu_x(\mathrm{d}s), \tag{2.8}$$

for a.a. $x\in\Omega$, all $\tilde\varrho \in (\varrho;+\infty]$, and all $v \in \mathcal{O}(\tilde\varrho)$ the following inequality is valid

$$Z^\infty v(\nabla u(x)) \le \int_{\mathbb{R}^{n\times n}_{\mathrm{inv}}} v(s)\nu_x(\mathrm{d}s). \tag{2.9}$$

Remark 2.6 It will follow from the proof of Theorem 2.5 that if $|\nabla u(x)| \le \varrho-\epsilon$ for some $\epsilon<\varrho$ and almost all $x\in\Omega$ then we can take $\tilde\varrho\ge\varrho$ in (2.9). Otherwise $\tilde\varrho>\varrho$ seems to be necessary, similarly as in [18].

If there is a convex compact $K \subset R^{n\times n}_\varrho$ such that $\operatorname{supp}\nu_x \subset K$ for almost all $x\in\Omega$ in Theorem 2.5 then it is sufficient to consider (2.9) only for all $v:\mathbb{R}^{n\times n}\to\mathbb{R}$ quasiconvex and bounded from below; cf. [26, Cor. 3]. In particular, either $K \subset R^{n\times n}_{\varrho+}$ or $\det A < 0$ for all $A\in K$. Assume that $K \subset R^{n\times n}_{\varrho+}$, i.e. $\det A > 0$ for all $A \in K$. Following [26, Cor. 3] we find a sequence $\{u_k\}_{k\in\mathbb{N}} \subset W^{1,\infty}(\Omega;\mathbb{R}^n)$ such that $\{\nabla u_k\}_{k\in\mathbb{N}}$ generates ν and $\|\mathrm{dist}(\nabla u_k, K)\|_{L^\infty} \to 0$ as $k\to\infty$. Hence, $\det\nabla u_k > 0$ for almost all $x\in\Omega$ if $k\ge k_0\in\mathbb{N}$ is large enough. This observation can be used in approximating minimizers of $\nu \mapsto \bar J(\nu) := \int_\Omega\int_{\mathbb{R}^{n\times n}_{\mathrm{inv}+}} W(A)\nu_x(\mathrm{d}A)\,\mathrm{d}x$.

3. Proofs in the L^p-case

This section is devoted to prove Theorems 2.1 and 2.2 when proving the necessity part of Theorem 2.1 by a combination of Propositions 3.3 and 3.5; the sufficiency part heavily relies on Proposition 3.6.

Proposition 3.1 *Let $\nu \in \mathcal{Y}(\Omega; \mathbb{R}^{n\times n})$ and suppose that there is $\varrho > 0$ such that for almost all $x \in \Omega$ supp $\nu_x \subset R_\varrho^{n\times n}$. Then there exists $\{Y_k\}_{k\in\mathbb{N}} \subset L^\infty(\Omega; \mathbb{R}^{n\times n})$ such that $\{Y_k(x)\}_{k\in\mathbb{N}} \subset R_\varrho^{n\times n}$ for almost all $x \in \Omega$ and $\{Y_k\}_{k\in\mathbb{N}}$ generates ν. The same result holds if we replace $R_\varrho^{n\times n}$ with $R_{\varrho+}^{n\times n}$.*

Proof This is a classical result mentioned in (1.11). See e.g. [12, Th. 1] for details. □

Proposition 3.2 *Let $\varrho > 0$ and let $\{Y_k\}_{k\in\mathbb{N}} \subset L^\infty(\Omega; \mathbb{R}^{n\times n})$, $\{Y_k\}_{k\in\mathbb{N}} \subset R_\varrho^{n\times n}$ for almost all $x \in \Omega$ and all $k \in \mathbb{N}$. If $\{Y_k\}_{k\in\mathbb{N}}$ generates $\nu \in \mathcal{Y}^\infty(\Omega; \mathbb{R}^{n\times n})$ and if $\{Y_k^{-1}\}_{k\in\mathbb{N}}$ generates $\mu \in \mathcal{Y}^\infty(\Omega; \mathbb{R}^{n\times n})$ then for almost all $x \in \Omega$ and every continuous $f : R_\varrho^{n\times n} \to \mathbb{R}$ it holds*

$$\int_{R_\varrho^{n\times n}} f(s)\mu_x(\mathrm{d}s) = \int_{R_\varrho^{n\times n}} f(s^{-1})\nu_x(\mathrm{d}s). \tag{3.1}$$

Moreover, supp $\nu_x \subset R_\varrho^{n\times n}$ *for almost all $x \in \Omega$. The same result holds for $R_{\varrho+}^{n\times n}$ instead of $R_\varrho^{n\times n}$.*

Proof First of all, recall that [27,28] for almost all $x \in \Omega$ ν_x is supported on the set $\cap_{l=1}^\infty \overline{\{Y_k(x);\ k \geq l\}}$, i.e. ν_x is supported on $R_\varrho^{n\times n}$. Further, notice that $\{Y_k^{-1}(x)\}_{k\in\mathbb{N}} \subset R_\varrho^{n\times n}$ for a.a. $x \in \Omega$. If $f : R_\varrho^{n\times n} \to \mathbb{R}$ is continuous, so is $F : R_\varrho^{n\times n} \to \mathbb{R}$, $F(s) := f(s^{-1})$. Then we have for any $g \in L^1(\Omega)$

$$\lim_{k\to\infty} \int_\Omega f(Y_k^{-1}(x))g(x)\,\mathrm{d}x = \int_\Omega \int_{R_\varrho^{n\times n}} f(s)\mu_x(\mathrm{d}s)g(x)\,\mathrm{d}x.$$

At the same time,

$$\begin{aligned}\lim_{k\to\infty} \int_\Omega F(Y_k(x))g(x)\,\mathrm{d}x &= \int_\Omega \int_{R_\varrho^{n\times n}} F(s)\nu_x(\mathrm{d}s)g(x)\,\mathrm{d}x\\ &= \int_\Omega \int_{R_\varrho^{n\times n}} f(s^{-1})\nu_x(\mathrm{d}s)g(x)\,\mathrm{d}x.\end{aligned}$$

Note that the above procedure stays valid for $R_{\varrho+}^{n\times n}$ instead of $R_\varrho^{n\times n}$. □

Proposition 3.3 *Let $\{Y_k\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{n\times n})$ generate $\nu \in \mathcal{Y}^p(\Omega; \mathbb{R}^{n\times n})$ and let $\int_\Omega |\det\, Y_k^{-1}|^q \mathrm{d}x \leq C$ for some $C > 0$ and some $q > 0$. Then*

$$\nu_x(\mathbb{R}^{n\times n} \setminus \mathbb{R}_{\mathrm{inv}}^{n\times n}) = 0 \quad \textit{for almost all} \quad x \in \Omega. \tag{3.2}$$

Moreover, if $\det Y_k > 0$ *a.e. in Ω then $\nu_x(\mathbb{R}^{n\times n} \setminus \mathbb{R}_{\mathrm{inv}+}^{n\times n}) = 0$.*

Proof Define $v : \mathbb{R}^{n\times n} \to [0; +\infty]$

$$v(Y) := \begin{cases} |\det\, Y^{-1}|^q & \text{if } Y \in \mathbb{R}_{\mathrm{inv}}^{n\times n},\\ +\infty & \text{otherwise.}\end{cases}$$

Then v is lower semicontinuous and by a fundamental result on Young measures (see e.g. [11, Th. 8.61]) we have that

$$\int_\Omega \int_{\mathbb{R}^{n\times n}} v(s)\nu_x(\mathrm{d}s)\,\mathrm{d}x \le \liminf_{k\to\infty} \int_\Omega v(Y_k(x))\,\mathrm{d}x = \liminf_{k\to\infty} \int_\Omega |\det\ Y_k^{-1}|^q\,\mathrm{d}x \le C,$$

which means that $\nu_x(\mathbb{R}^{n\times n} \setminus \mathbb{R}^{n\times n}_{\rm inv}) = 0$ for almost all $x \in \Omega$. To prove the second claim, we argue the same way with a re-defined function $v : \mathbb{R}^{n\times n} \to [0; +\infty]$

$$v(Y) := \begin{cases} |\det\ Y^{-1}|^q & \text{if } \det Y > 0, \\ +\infty & \text{otherwise.} \end{cases}$$

□

Lemma 3.4 *Let $\nu \in \mathcal{Y}^{p,-p}(\Omega; \mathbb{R}^{n\times n})$, $\mu \in \mathcal{Y}^{p,-p}(\Omega; \mathbb{R}^{n\times n})$. Let $f \in C^{p,-p}(\mathbb{R}^{n\times n}_{\rm inv})$. Let also,*

$$\int_\Omega \int_{\mathbb{R}^{n\times n}_{\rm inv}} f^\varrho(s)\mu_x(\mathrm{d}s)\,\mathrm{d}x = \int_\Omega \int_{\mathbb{R}^{n\times n}_{\rm inv}} f^\varrho(s^{-1})\nu_x(\mathrm{d}s)\mathrm{d}x \tag{3.3}$$

for all $f^\varrho \in \{h \in C_0(\mathbb{R}^{n\times n});\ \mathrm{supp}\, h\ \subset R^{n\times n}_\varrho\}$, for any $\varrho > 0$. Then

$$\int_\Omega \int_{\mathbb{R}^{n\times n}_{\rm inv}} f(s)\mu_x(\mathrm{d}s)\mathrm{d}x = \int_\Omega \int_{\mathbb{R}^{n\times n}_{\rm inv}} f(s^{-1})\nu_x(\mathrm{d}s)\mathrm{d}x\ . \tag{3.4}$$

Proof The proof is a simple application of suitable cut-off functions and of Lebesgue's dominated convergence theorem. □

Proposition 3.5 *Let $p \in [1, \infty)$ and $\{Y_k\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{n\times n})$, $\{Y_k^{-1}\}_{k\in\mathbb{N}} \subset L^p(\Omega; R^{n\times n})$ be bounded. Then there is a (not relabelled) subsequence of $\{Y_k\}_{k\in\mathbb{N}}$ generating a Young measure $\nu \in \mathcal{Y}^{p,-p}(\Omega; \mathbb{R}^{n\times n})$.*

Moreover, if we denoted μ the Young measure generated by (a further subsequence of) $\{Y_k^{-1}\}_{k\in\mathbb{N}}$ then (3.4) *holds for all $f \in C^{p,-p}(\mathbb{R}^{n\times n}_{\rm inv})$.*

Proof It follows from (1.12) that a (not relabelled) subsequence of $\{Y_k\}_{k\in\mathbb{N}}$ generates a Young measure $\nu \in \mathcal{Y}^p(\Omega; \mathbb{R}^{n\times n})$ and $\{Y_k^{-1}\}_{k\in\mathbb{N}}$ generates a Young measure $\mu \in \mathcal{Y}^p(\Omega; \mathbb{R}^{n\times n})$. As $\int_\Omega |\det (Y_k^{-1})|^{p/n}\mathrm{d}x \le C \int_\Omega |Y_k^{-1}|^p\mathrm{d}x < +\infty$, we know from Proposition 3.3 that ν_x and μ_x are both supported on $\mathbb{R}^{n\times n}_{\rm inv}$ for almost all $x \in \Omega$. We have for all $g \in L^\infty(\Omega)$ and all $v \in C_0(\mathbb{R}^{n\times n})$

$$\lim_{k\to\infty} \int_\Omega v(Y_k^{-1}(x))g(x)\,\mathrm{d}x = \int_\Omega \int_{\mathbb{R}^{n\times n}_{\rm inv}} v(s^{-1})\nu_x(\mathrm{d}s)g(x)\,\mathrm{d}x,$$

$$\lim_{k\to\infty} \int_\Omega v(Y_k^{-1}(x))g(x)\,\mathrm{d}x = \int_\Omega \int_{\mathbb{R}^{n\times n}_{\rm inv}} v(s)\mu_x(\mathrm{d}s)g(x)\,\mathrm{d}x.$$

This means that for all $g \in L^\infty(\Omega)$ and all $v \in C_0(\mathbb{R}^{n\times n})$

$$\int_\Omega \int_{\mathbb{R}^{n\times n}_{\rm inv}} v(s^{-1})\nu_x(\mathrm{d}s)g(x)\,\mathrm{d}x = \int_\Omega \int_{\mathbb{R}^{n\times n}_{\rm inv}} v(s)\mu_x(\mathrm{d}s)g(x)\,\mathrm{d}x; \tag{3.5}$$

in particular, the equality holds for all v supported on $R^{n\times n}_\varrho$.

It remains only to prove that $\int_\Omega \int_{\mathbb{R}^{n\times n}_{\text{inv}}} (|s|^p + |s^{-1}|^p)\nu_x(\mathrm{d}s)\mathrm{d}x$ is bounded. This can be shown by an application of [11, Th. 8.61], similarly as in the proof of Proposition 3.3, when setting $s^{-1} = +\infty$ in singular matrices. Note that, since ν_x is supported on invertible matrices, this extension will not play a role.

Therefore, by Lemma 3.4, (3.4) holds for all $f \in C^{p,-p}(\mathbb{R}^{n\times n}_{\text{inv}})$. □

Proposition 3.6 *Let $\nu \in \mathcal{Y}^{p,-p}(\Omega; \mathbb{R}^{n\times n})$. Then there is a generating sequence $\{Y_k\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{n\times n})$ such that $\{Y_k^{-1}\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{n\times n})$ is bounded. Moreover, $\{|Y_k^{-1}|^p\}_{k\in\mathbb{N}}$ as well as $\{|Y_k|^p\}_{k\in\mathbb{N}}$ are equi-integrable.*

Proof Notice that inevitably supp $\nu_x \subset \mathbb{R}^{n\times n}_{\text{inv}}$ for a.a. $x \in \Omega$ (cf. (2.1)). Therefore, we define smooth cut-off functions Φ_ϱ which are 1 on $R^{n\times n}_\varrho$ and 0 on $\mathbb{R}^{n\times n}_{\text{inv}} \setminus R^{n\times n}_{\varrho+1}$; note that Φ_ϱ can be found as follows: construct Θ_ϱ a smooth function which is 1 inside the ball $B(0,\varrho) \subset \mathbb{R}^{n\times n}$ and equals 0 on $\mathbb{R}^{n\times n} \setminus B(0,\varrho+1)$. Now, we may set $\Phi_\varrho(s) := \Theta_\varrho(s)\Theta_\varrho(s^{-1})$. Then, we define

$$\nu_x^\varrho \ := \ \Phi_\varrho \nu_x + \left(\int_{\mathbb{R}^{n\times n}_{\text{inv}}} \left(1 - \Phi_\varrho(s)\right) \nu_x(\mathrm{d}s) \right) \delta_I, \tag{3.6}$$

where δ_I denotes the Dirac measure supported at the identity matrix. It is a simple observation that $\{\nu_x^\varrho\}_{x\in\Omega} =: \nu^\varrho \in \mathcal{Y}(\Omega; \mathbb{R}^{n\times n})$ such that supp $\nu_x^\varrho \subset R^{n\times n}_{\varrho+1}$ for a.e. $x \in \Omega$.

Due to Propositions 3.1 and 3.2, there exists $\{Y_k^\varrho\}_{k\in\mathbb{N}} \subset R^{n\times n}_{\varrho+1}$ with $\{(Y_k^\varrho)^{-1}\}_{k\in\mathbb{N}} \subset R^{n\times n}_{\varrho+1}$ for a.e. $x \in \Omega$ generating ν^ϱ and μ^ϱ, respectively, that satisfy for all $v \in C_0(\mathbb{R}^{n\times n})$

$$\int_{\mathbb{R}^{n\times n}_{\text{inv}}} v(s^{-1})\nu_x^\varrho(\mathrm{d}s) = \int_{\mathbb{R}^{n\times n}_{\text{inv}}} v(s)\mu_x^\varrho(\mathrm{d}s). \tag{3.7}$$

Now, for any $g \in L^\infty(\Omega)$ we can write

$$\begin{aligned} \lim_{\varrho\to\infty} \int_\Omega g(x) \int_{\mathbb{R}^{n\times n}_{\text{inv}}} v(s)\nu_x^\varrho(\mathrm{d}s)\mathrm{d}x \\ = \lim_{\varrho\to\infty} \int_\Omega g(x) \int_{\mathbb{R}^{n\times n}_{\text{inv}}} v(s)\Phi_\varrho(s)\nu_x(\mathrm{d}s)\mathrm{d}x \\ + \lim_{\varrho\to\infty} v(I) \int_\Omega g(x) \int_{\mathbb{R}^{n\times n}_{\text{inv}}} (1 - \Phi_\varrho(s))\nu_x(\mathrm{d}s)\mathrm{d}x. \end{aligned}$$

As $v\Phi_\varrho$ converges strongly in the C_0-norm to v and $\int_{\mathbb{R}^{n\times n}_{\text{inv}}}(1 - \Phi_\varrho(s))\nu_x(\mathrm{d}s)$ converges to 0 for a.e. $x \in \Omega$, thanks to Lebesgue's dominated convergence theorem, we are in the situation that

$$\lim_{\varrho\to\infty} \lim_{k\to\infty} v(Y_k^\varrho) = \int_{\mathbb{R}^{n\times n}_{\text{inv}}} v(s)\nu_x(\mathrm{d}s) \text{ weakly in } L^1(\Omega).$$

Further, we verify that $\{Y_k^\varrho\}_{k\in\mathbb{N}}$ as well as $\{(Y_k^\varrho)^{-1}\}_{k\in\mathbb{N}}$ are bounded in $L^p(\Omega; \mathbb{R}^{n\times n})$ independently of ϱ. Indeed, for every $\varrho \geq 1$ fixed we have that,

$$\begin{aligned} \lim_{k\to\infty} \int_\Omega |Y_k^\varrho|^p \,\mathrm{d}x &= \int_\Omega \int_{\mathbb{R}^{n\times n}_{\text{inv}}} |s|^p \,\nu_x^\varrho(\mathrm{d}s)\,\mathrm{d}x \\ &\leq \int_\Omega \int_{B(0,\varrho+1)} |s|^p \nu_x(\mathrm{d}s)\,\mathrm{d}x \leq \int_\Omega \int_{\mathbb{R}^{n\times n}_{\text{inv}}} |s|^p \,\nu_x(\mathrm{d}s)\,\mathrm{d}x \leq C; \end{aligned} \tag{3.8}$$

an analogous calculation could be carried out for $\{(Y_k^{\varrho})^{-1}\}_{k\in\mathbb{N}}$.

Applying the diagonalization argument (as $L^1(\Omega; C_0(\mathbb{R}^{n\times n}))$ is separable) we get a sequence $\{Y_k\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{n\times n})$ generating ν that is, thanks to (3.8), also equi-integrable; the same holds for the inverse.

Moreover, if we defined μ as the weak* limit of μ_ϱ, then μ would be generated by $\{Y_k^{-1}\}_{k\in\mathbb{N}} \subset L^p(\Omega; \mathbb{R}^{n\times n})$ as, due to its definition,

$$\lim_{\varrho\to\infty}\lim_{k\to\infty} v((Y_k^{\varrho})^{-1}) = \int_{\mathbb{R}^{n\times n}_{\rm inv}} v(s)\mu_x(\mathrm{d}s) \text{ weakly in } L^1(\Omega)\,.$$

Also, by applying $\varrho \to \infty$ in (3.7), it holds that

$$\int_{\mathbb{R}^{n\times n}_{\rm inv}} v(s^{-1})\nu_x(\mathrm{d}s) = \int_{\mathbb{R}^{n\times n}_{\rm inv}} v(s)\mu_x(\mathrm{d}s), \tag{3.9}$$

for all $v \in C_0(\mathbb{R}^{n\times n})$ and hence, by Lemma 3.4, also for all $v \in C^{p,-p}(\mathbb{R}^{n\times n}_{\rm inv})$. □

Proof of Theorem 2.1. The necessity part follows from Propositions 3.3 and 3.5 while the sufficiency part follows from Proposition 3.6.

It thus remains to prove relation (2.3), which can be proven analogously to [11, Th. 8.6]; however, we need to show that if $f(x,s) = g(x)v(s)$ for some $g \in L^\infty(\Omega)$ and $v \in C_{p,-p}(\mathbb{R}^{n\times n}_{\rm inv})$ then $\{f(x, Y_k(x))\}_{k\in\mathbb{N}}$ is equi-integrable. To see this, we use [30, Lemma 6.1] and show only that for every $\varepsilon > 0$ there exists $K > 0$ such that $\int_{\{x\in\Omega;|v(Y_k(x))|\geq K\}} |v(Y_k(x))|\,\mathrm{d}x \leq \varepsilon$.

Notice that there exists $C > 0$ such that $v_0(s) := |v(s)|/(|s|^p + |s^{-1}|^p) \leq C$ for every $s \in \mathbb{R}^{n\times n}_{\rm inv}$. Moreover, $\lim_{|s|^p+|s^{-1}|^p\to\infty} v_0(s) = 0$. Let $(\|Y_k\|^p_{L^p} + \|Y_k^{-1}\|^p_{L^p}) \leq M$ and take $\varepsilon > 0$ and $K > 0$ large enough so that $|v_0(s)| < \varepsilon/M$ if $|s|^p + |s^{-1}|^p \geq K/C$. Then for all k

$$\begin{aligned}
\int_{\{x\in\Omega;\ |v(Y_k(x))|\geq K\}} |v(Y_k(x))|\,\mathrm{d}x &\leq \int_{\{x\in\Omega;\ |Y_k(x)|^p+|(Y_k(x))^{-1}|^p\geq K/C\}} |v(Y_k(x))|\,\mathrm{d}x\\
&\leq \int_{\{x\in\Omega;|Y_k(x)|^p+|Y_k^{-1}(x)|^p\geq K/C\}} |v_0(Y_k(x))|(|Y_k(x)|^p + |Y_k^{-1}(x)|^p)\mathrm{d}x\\
&\leq \varepsilon/M ? \int_\Omega |Y_k(x)|^p + |Y_k^{-1}(x)|^p\mathrm{d}x \leq \varepsilon.
\end{aligned}$$

□

Proof of Theorem 2.2. It is analogous to the proof of Theorem 2.1. Notice that ν is supported on matrices with positive determinant due to Proposition 3.3. The converse implication follows from Proposition 3.1. □

Proof of Proposition 2.4. By the Mazur lemma $\det \nabla y \geq 0$. Suppose, by contradiction, there existed a set $\omega \subset \Omega$ of non-zero Lebesgue measure such that $\det \nabla y = 0$ on ω. We have by the sequential weak continuity of $y \mapsto \det \nabla y$ from $W^{1,p}(\Omega; \mathbb{R}^n)$ to $L^{p/n}(\Omega)$ [2] that

$$\int_\omega |\det \nabla y_k(x)|\,\mathrm{d}x = \int_\omega \det \nabla y_k(x)\,\mathrm{d}x \to 0 \text{ as } k \to \infty,$$

so, it holds for a subsequence (not relabelled) that $0 < \det \nabla y_k \to 0$ a.e. in ω. By the Fatou lemma, we have

$$\int_\omega \liminf_{k\to\infty} \frac{\mathrm{d}x}{\det \nabla y_k(x)} \le \liminf_{k\to\infty} \int_\omega \frac{\mathrm{d}x}{\det \nabla y_k(x)} \le C \liminf_{k\to\infty} \int_\omega |(\nabla y_k(x))^{-1}|^n \,\mathrm{d}x,$$

however, the left-hand side tends to $+\infty$. This contradicts the boundedness of $\{(\nabla y_k)^{-1}\}_{k\in\mathbb{N}}$ in $L^p(\Omega;\mathbb{R}^{n\times n})$ because $p > n$ and Ω is bounded. Hence, $\det \nabla y > 0$ a.e. in Ω. The assertion about the support follows from Proposition 3.3. □

4. Proofs in the $W^{1,\infty}$-case

We shall heavily rely on the following convex integration result which can be found in [29, p. 199 and Remark 2.4]; recall that $O(n)$ will standardly denote the set of orthogonal matrices in $\mathbb{R}^{n\times n}$, i.e. $O(n) := \{A \in \mathbb{R}^{n\times n};\ A^\top A = AA^\top = I\}$.

LEMMA 4.1 *Let $\omega \subset \mathbb{R}^n$ be open and Lipschitz. Let $\varphi \in W^{1,\infty}(\omega;\mathbb{R}^n)$ be such that there is $\vartheta > 0$, so that $0 \le |\nabla\varphi| \le 1-\vartheta$ a.e. in ω. Then there exist mappings $u \in W^{1,\infty}(\omega;\mathbb{R}^n)$ for which $\nabla u \in O(n)$ 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 $\{\psi := z+\varphi;\ z \in W^{1,\infty}_0(\omega;\mathbb{R}^n)\ ,\ |\nabla\psi| \le 1-\vartheta$ a.e. in $\omega\}$.*

Before proving Theorem 2.5, let us elaborate more on the connection of the envelope $Z^\infty v$ from (1.10) and the standard quasi-convex envelope. If $v \in \mathcal{O}(\varrho)$ with $\varrho < \infty$ it is not clear whether $Z^\infty v$ is quasiconvex. However, this holds in the case when $\rho = +\infty$ as the following proposition shows.

PROPOSITION 4.2 *Let $v : \mathbb{R}^{n\times n} \to \mathbb{R}\cup\{+\infty\}$ be in $\mathcal{O}(+\infty)$. Then $Z^\infty v = Qv$.*

Proof Let us establish that $Z^\infty v(A) < +\infty$ for all $A \in \mathbb{R}^{n\times n}$. This is clear if $A \in \mathbb{R}^{n\times n}_{\mathrm{inv}}$, otherwise we use Lemma 4.1 to construct $\psi \in W^{1,\infty}_A(\Omega;\mathbb{R}^n)$ and $\nabla\psi \in (|A|+\varepsilon)O(n)$ for some $\varepsilon > 0$. Thus, $|\Omega| Z^\infty v(A) \le \int_\Omega v(\nabla\psi(A))\,\mathrm{d}x < +\infty$.

Due to the finiteness of $Z^\infty v$, we know by [31, Thm. 2.4] that $Z^\infty v = Qv$, i.e. $Z^\infty v$ is quasiconvex and continuous. □

4.1. *Proof of Theorem 2.5 – necessity*

Conditions (2.7) and (2.8) are standard we only need to prove (2.9).

PROPOSITION 4.3 *Let $F \in \mathbb{R}^{n\times n}$, $u_F(x) := Fx$ if $x \in \Omega$, $y_k \overset{*}{\rightharpoonup} u_F$ in $W^{1,\infty}(\Omega;\mathbb{R}^n)$ and let for some $\alpha > 0$ $\nabla y_k(x) \in R^{n\times n}_\alpha$ for all $k > 0$ and almost all $x \in \Omega$. Then for every $\varepsilon > 0$ there is $\{u_k\}_{k\in\mathbb{N}} \subset W^{1,\infty}(\Omega;\mathbb{R}^n)$ such that $\nabla u_k(x) \in R^{n\times n}_{\alpha+\varepsilon}$ for all $k > 0$ and almost all $x \in \Omega$, $u_k - u_F \in W^{1,\infty}_0(\Omega;\mathbb{R}^n)$ and $|\nabla y_k - \nabla u_k| \to 0$ in measure. In particular, $\{\nabla y_k\}_{k\in\mathbb{N}}$ and $\{\nabla u_k\}_{k\in\mathbb{N}}$ generate the same Young measure.*

Proof Define for $\ell > 0$, sufficiently large, $\Omega_\ell := \{x \in \Omega;\ \mathrm{dist}(x,\partial\Omega) \ge 1/\ell\}_{\ell\in\mathbb{N}}$ and 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 $C > 0$. Set $z_{k\ell} := \eta_\ell y_k + (1-\eta_\ell)u_F$. Then $z_{k\ell} \in W^{1,\infty}(\Omega;\mathbb{R}^n)$ and $z_{k\ell} = y_k$ in Ω_ℓ and $z_{k\ell} = u_F$ on $\partial\Omega$. We see that $\nabla z_{k\ell} = \eta_\ell\nabla y_k + (1-\eta_\ell)F + (y_k - u_F)\otimes\nabla\eta_\ell$. Hence, in view of the facts that $|F| \le \liminf_{k\to\infty}\|\nabla y_k\|_{L^\infty} \le \alpha$ and that $y_k \to u_F$ uniformly in $\overline{\Omega}$, we can extract for every $\varepsilon > 0$ a (not relabelled) subsequence $k = k(\ell)$ such that

$$\|\nabla z_{k(\ell)\ell}\|_{L^\infty} < \alpha + \frac{\varepsilon}{2}.$$

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

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

Let us denote $\omega_\ell := \Omega\setminus\Omega_\ell$, then $w_{k(\ell)\ell} := z_{k(\ell)\ell\ \omega_\ell}/(\alpha+\varepsilon)$ is such that $|\nabla w_{k(\ell)\ell}| \le 1-\vartheta$ for $\vartheta := \varepsilon/2(\alpha+\varepsilon)$. We use Lemma 4.1 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 $\{u_{k(\ell)\ell}\}_{\ell\in\mathbb{N}} \subset W^{1,\infty}(\Omega;\mathbb{R}^n)$ and that $u_{k(\ell)\ell}(x) = Fx$ for $x \in \partial\Omega$. Further, $\nabla u_{k(\ell)\ell}(x) \in R^{n\times n}_{\alpha+\varepsilon}$. Moreover, the Lebesgue measure of $\{x \in \Omega;\ \nabla u_{k(\ell)\ell}(x) \ne \nabla y_k(x)\}$ vanishes if $k \to \infty$ and $\ell \to \infty$ sufficiently fast, therefore both sequences generate the same Young measure by [30, Lemma 8.3]. □

Remark 4.4
(i) It follows from the above proof that if $|F| < \alpha$ then we can take $\varepsilon = 0$ in Proposition 4.3.
(ii) If $\{u_k\}_{k\in\mathbb{N}}$ defined in the proof of Proposition 4.3 are homeomorphic and $n = 2$ then either $\det\nabla u_k > 0$ or $\det\nabla u_k < 0$ in Ω for all k. The reason is that homeomorphisms in two dimensions are either orientation preserving or reversing.

LEMMA 4.5 *Let $\nu \in \mathcal{GY}^{+\infty,-\infty}_\varrho(\Omega;\mathbb{R}^{n\times n})$. Then $\mu := \{\nu_a\}_{x\in\Omega} \in \mathcal{GY}^{+\infty,-\infty}_\varrho(\Omega;\mathbb{R}^{n\times n})$ for a.e. $a \in \Omega$.*

Proof Note that the construction in the proof of [30, Th. 7.2] does not affect invertibility. □

PROPOSITION 4.6 *Let $\nu \in \mathcal{GY}^{+\infty,-\infty}(\Omega;\mathbb{R}^{n\times n})$, $\operatorname{supp}\nu \subset R^{n\times n}_\varrho$ be such that for almost all $x \in \Omega$ $\nabla y(x) = \int_{R^{n\times n}_\varrho} s\nu_x(\mathrm{d}s)$, where $y \in W^{1,\infty}(\Omega;\mathbb{R}^n)$. Then for all $\tilde\varrho \in (\varrho;+\infty]$, almost all $x \in \Omega$ and all $v \in \mathcal{O}(\tilde\varrho)$ we have*

$$\int_{\mathbb{R}^{n\times n}_{\mathrm{inv}}} v(s)\nu_x(\mathrm{d}s) \ge Z^\infty v(\nabla y(x)). \tag{4.1}$$

Proof We know from Lemma 4.5 that $\mu = \{\nu_a\}_{x\in\Omega} \in \mathcal{GY}^{+\infty,-\infty}_\varrho(\Omega;\mathbb{R}^{n\times n})$ for a.e. $a \in \Omega$, so there exits its generating sequence $\{\nabla u_k\}_{k\in\mathbb{N}}$ such that $\{u_k\}_{k\in\mathbb{N}} \subset W^{1,\infty}(\Omega;\mathbb{R}^n)$ and for almost all $x \in \Omega$ and all $k \in \mathbb{N}$ $\nabla u_k(x) \in R^{n\times n}_\varrho$. Moreover, $\{u_k\}_{k\in\mathbb{N}}$ weakly* converges to the map $x \mapsto (\nabla y(a))x$.

Using Proposition 4.3, we can, without loss of generality, suppose that $\nabla u_k \in R^{n\times n}_{\tilde{\varrho}}$ for all $k \in \mathbb{N}$ and $u_k(x) = \nabla y(a)x$ if $x \in \partial\Omega$. Therefore, we have

$$|\Omega| \int_{\mathbb{R}^{n\times n}_{\rm inv}} v(s)\nu_a(\mathrm{d}s) = \lim_{k\to\infty} \int_\Omega v(\nabla u_k(x))\,\mathrm{d}x \geq |\Omega| Z^\infty v(\nabla y(a)).$$

□

4.2. *Proof of Theorem 2.5 – sufficiency*

We need to show that conditions (2.7),(2.8), and (2.9) are also sufficient for $\nu \in \mathrm{rca}(\mathbb{R}^{n\times n}_{\rm inv})$ to be in $\mathcal{GY}^{+\infty,-\infty}(\Omega;\mathbb{R}^{n\times n})$. Put

$$\mathcal{U}^\varrho_A := \{y \in W^{1,\infty}_A(\Omega;\mathbb{R}^n);\ \nabla y \in R^{n\times n}_\varrho\}. \tag{4.2}$$

Consider for $A \in \mathbb{R}^{n\times n}$ the set

$$\mathcal{M}^\varrho_A := \{\overline{\delta_{\nabla y}};\ y \in \mathcal{U}^\varrho_A\}\,, \tag{4.3}$$

where $\overline{\delta_{\nabla y}} \in \mathrm{rca}(\mathbb{R}^{n\times n})$ is defined as $\langle\overline{\delta_{\nabla y}}, v\rangle := |\Omega|^{-1}\int_\Omega v(\nabla y(x))\,\mathrm{d}x$; $\overline{\mathcal{M}^\varrho_A}$ will denote its weak* closure.

We have the following lemma:

Lemma 4.7 *Let $A \in \mathbb{R}^{n\times n}$ If $\varrho > |A|$ then the set $\mathcal{M}^\varrho_A$ is nonempty and convex.*

Proof First we show that $\mathcal{M}^\varrho_A$ is non-empty. This is clear when A is invertible. Otherwise, note that $|A|/\varrho = 1 - (\varrho - |A|)/\varrho$. Thus, we can apply Lemma 4.1 with $\varphi(x) := Ax/\varrho$, $x \in \Omega$ and $\vartheta := (\varrho - |A|)/\varrho$ to get $u \in W^{1,\infty}(\Omega;\mathbb{R}^n)$ such that $\nabla u \in O(n)$ a.e. in Ω and $u(x) = Ax/\varrho$ if $x \in \partial\Omega$. Therefore, $y := \varrho u \in \mathcal{U}^\varrho_A$. Consequently, $\mathcal{M}^\varrho_A \neq \emptyset$.

The rest of proof is analogous to the proof of [30, Lemma 8.5]. We take $y_1, y_2 \in \mathcal{U}^\varrho_A$ and, for a given $\lambda \in (0,1)$, we find a subset $D \subset \Omega$ such that $|D| = \lambda|\Omega|$. There are two countable families of subsets of D and $\Omega \setminus D$ of the form

$$\{a_i + \epsilon_i\Omega;\ a_i \in D,\ \epsilon_i > 0,\ a_i + \epsilon_i\Omega \subset D\}$$

and

$$\{b_i + \epsilon_i\Omega;\ b_i \in \Omega\setminus D,\ \rho_i > 0,\ b_i + \rho_i\Omega \subset \Omega \setminus D\}$$

such that

$$D = \cup_i(a_i + \epsilon_i\Omega) \cup N_0, \qquad \Omega\setminus D = \cup_i(b_i + \rho_i\Omega) \cup N_1,$$

where the Lebesgue measure of N_0 and N_1 is zero. We define

$$y(x) := \begin{cases} \epsilon_i y_1\left(\frac{x-a_i}{\epsilon_i}\right) + Aa_i & \text{if } x \in a_i + \epsilon_i\Omega,\\ \rho_i y_2\left(\frac{x-b_i}{\rho_i}\right) + Ab_i & \text{if } x \in b_i + \rho_i\Omega,\\ Ax & \text{otherwise,}\end{cases}$$

yielding

$$\nabla y(x) = \begin{cases} \nabla y_1\left(\frac{x-a_i}{\epsilon_i}\right) & \text{if } x \in a_i + \epsilon_i\Omega,\\ \nabla y_2\left(\frac{x-b_i}{\rho_i}\right) & \text{if } x \in b_i + \rho_i\Omega,\\ A & \text{otherwise.}\end{cases}$$

In particular, $y \in \mathcal{U}_A^\varrho$ and $\overline{\delta_{\nabla y}} = \lambda \overline{\delta_{\nabla y_1}} + (1-\lambda)\overline{\delta_{\nabla y_2}}$. □

The following homogenization lemma can be proved the same way as [30, Th. 7.1].

LEMMA 4.8 *Let $\{u_k\}_{k\in\mathbb{N}} \subset W_A^{1,\infty}(\Omega;\mathbb{R}^n)$ be a bounded sequence such that $\{\nabla u_k\}_{k\in\mathbb{N}}$ are invertible and $\{(\nabla u_k)^{-1}\}_{k\in\mathbb{N}} \subset L^\infty(\Omega;\mathbb{R}^{n\times n})$ bounded. Let $\nu \in \mathcal{GY}^{+\infty,-\infty}(\Omega;\mathbb{R}^{n\times n})$ be generated by $\{\nabla u_k\}_{k\in\mathbb{N}}$. Then there is a bounded sequence $\{w_k\}_{k\in\mathbb{N}} \subset W_A^{1,\infty}(\Omega;\mathbb{R}^n)$ with $\{\nabla w_k\}_{k\in\mathbb{N}}$ invertible and $\{(\nabla w_k)^{-1}\}_{k\in\mathbb{N}} \subset L^\infty(\Omega;\mathbb{R}^{n\times n})$ bounded such that $\{\nabla w_k\}_{k\in\mathbb{N}}$ generates $\overline{\nu} \in \mathcal{GY}^{+\infty,-\infty}(\Omega;\mathbb{R}^{n\times n})$ defined through*

$$\int_{\mathbb{R}^{n\times n}} v(s)\overline{\nu}_x(\mathrm{d}s) = \frac{1}{|\Omega|}\int_\Omega \int_{\mathbb{R}^{n\times n}} v(s)\nu_x(\mathrm{d}s)\,\mathrm{d}x, \tag{4.4}$$

for any $v \in C_0(\mathbb{R}^{n\times n})$ and almost all $x \in \Omega$.

PROPOSITION 4.9 *Let μ be a probability measure supported on a compact set $K \subset \mathbb{R}_\alpha^{n\times n}$ for some $\alpha \geq 1$ and let $A := \int_K s\mu(\mathrm{d}s)$. Let $\varrho > \alpha$ and let*

$$Z^\infty v(A) \leq \int_K v(s)\mu(\mathrm{d}s), \tag{4.5}$$

for all $v \in \mathcal{O}(\varrho)$. Then $\mu \in \mathcal{GY}^{+\infty,-\infty}(\Omega;\mathbb{R}^{n\times n})$ and it is generated by gradients of mappings from $\mathcal{U}_A^\varrho$.

Proof The proof standardly uses the Hahn–Banach theorem and Lemma 4.8 and it is similar to [30, Proposition 8.17]. First, notice that $|A| \leq \alpha < \varrho < +\infty$. Then, since $\mathcal{M}_A^\varrho$ is non-empty and convex due to Lemma 4.7, we can, by the Hahn–Banach theorem, assume that there is $\tilde{v} \in C(R_\varrho^{n\times n})$ such that

$$0 \leq \langle \nu, \tilde{v}\rangle = \int_{R_\varrho^{n\times n}} \tilde{v}(s)\nu(\mathrm{d}s) = |\Omega|^{-1}\int_\Omega \tilde{v}(\nabla y(x))\,\mathrm{d}x,$$

for all $\nu \in \mathcal{M}_A^\varrho$, and hence all $y \in \mathcal{U}_A^\varrho$, and $0 > \langle \tilde{\nu}, \tilde{v}\rangle$ if $\tilde{\nu} \in \mathrm{rca}(\mathbb{R}^{n\times n}) \setminus \overline{\mathcal{M}_A^\varrho}$.

Now, the function

$$\bar{v}(F) := \begin{cases} \tilde{v}(F) & \text{if } F \in R_\varrho^{n\times n}, \\ +\infty & \text{else,} \end{cases}$$

is in $\mathcal{O}(\varrho)$. Notice that it follows from (4.5) that $Z^\infty \bar{v}(A)$ is finite. Thus, $Z^\infty v(A) = \inf_{\mathcal{U}_A^\varrho} |\Omega|^{-1}\int_\Omega v(\nabla y(x))\,\mathrm{d}x$ and hence $Z^\infty v(A) \geq 0$ and, by (4.5), $0 \leq \int_{R_\varrho^{n\times n}} v(s)\mu(\mathrm{d}s)$. Thus, $\mu \in \overline{\mathcal{M}_A^\varrho}$. As $C(R_\varrho^{n\times n})$ is separable, the weak* topology on bounded sets in $\mathrm{rca}(R_\varrho^{n\times n})$ is metrizable. Hence, there is a sequence $\{u_k\}_{k\in\mathbb{N}} \subset \mathcal{U}_A^\varrho$ such that for all $v \in C(R_\varrho^{n\times n})$ (and all $v \in \mathcal{O}(\varrho)$)

$$\lim_{k\to\infty}\int_\Omega v(\nabla u_k(x))\,\mathrm{d}x = |\Omega|\int_{R_\varrho^{n\times n}} v(s)\mu(\mathrm{d}s),$$

and $\{u_k\}_{k\in\mathbb{N}}$ is bounded in $W^{1,\infty}(\Omega;\mathbb{R}^{n\times n})$ due to the Poincaré inequality. As $u_k(x) = Ax$ for $x \in \partial\Omega$ we use the homogenization procedure from Lemma 4.8 to show that μ is the homogeneous Young measure generated by $\{\nabla u_k\}_{k\in\mathbb{N}}$. □

We will need the following auxiliary result.

LEMMA 4.10 (see [18, Lemma 6.1]) *Let $\Omega \subset \mathbb{R}^n$ be an open domain with $|\partial\Omega| = 0$ and let $N \subset \Omega$ be of the zero Lebesgue measure. For $r_k : \Omega \setminus N \to (0, +\infty)$ and $\{f_j\}_{j\in\mathbb{N}} \subset L^1(\Omega)$ there exists a set of points $\{a_{ik}\}_{i\in\mathbb{N}} \subset \Omega \setminus N$ and positive numbers $\{\epsilon_{ik}\}_{i\in\mathbb{N}}$, $\epsilon_{ik} \le r_k(a_{ik})$ such that $\{a_{ik} + \epsilon_{ik}\bar{\Omega}\}_{i\in\mathbb{N}}$ are pairwise disjoint for each $k \in \mathbb{N}$, $\bar{\Omega} = \cup_i\{a_{ik} + \epsilon_{ik}\bar{\Omega}\} \cup N_k$ with $|N_k| = 0$ and for any $j \in \mathbb{N}$*

$$\lim_{k\to\infty} \sum_i f_j(a_{ik})|\epsilon_{ik}\Omega| = \int_\Omega f_j(x)\,\mathrm{d}x.$$

Proof of Theorem 2.5 – sufficiency. Some parts of the proof follow [18, Proof of Th. 6.1]. We are looking for a sequence $\{u_k\}_{k\in\mathbb{N}} \subset W^{1,\infty}(\Omega;\mathbb{R}^n)$ with $\{\nabla u_k\}_{k\in\mathbb{N}}$ invertible and $\{(\nabla u_k)^{-1}\}_{k\in\mathbb{N}} \subset L^\infty(\Omega;\mathbb{R}^{n\times n})$ satisfying

$$\lim_{k\to\infty} \int_\Omega v(\nabla u_k(x))g(x)\,\mathrm{d}x = \int_\Omega \int_{\mathbb{R}^{n\times n}} v(s)\nu_x(\mathrm{d}s)g(x)\,\mathrm{d}x$$

for all $g \in \Gamma$ and any $v \in S$, where Γ and S are countable dense subsets of $C(\bar{\Omega})$ and $C_0(\mathbb{R}^{n\times n})$, respectively.

First of all notice that, as $u \in W^{1,\infty}(\Omega;\mathbb{R}^n)$ from (2.8) is differentiable in Ω outside a set of measure zero called N, we may find for every $a \in \Omega \setminus N$ and every $k > 0$ a $r_k(a) > 0$ such that for any $0 < \epsilon < r_k(a)$ we have

$$\frac{1}{\epsilon}|u(a+\epsilon y) - u(a) - \epsilon\nabla u(a)y| \le \frac{1}{k}. \tag{4.6}$$

Furthermore, as g is continuous, we choose $r_k(a) > 0$ smaller if necessary to assure that for any $0 < \epsilon < r_k(a)$

$$\left|\int_{a+\epsilon\Omega} g(x)\,\mathrm{d}x - g(a)\epsilon\right| < \frac{1}{k}. \tag{4.7}$$

From Lemma 4.10 we can find $a_{ik} \in \Omega \setminus N$, $\epsilon_{ik} \le r_k(a_{ik})$ such that for all $v \in S$ and all $g \in \Gamma$

$$\lim_{k\to\infty} \sum_i \bar{V}(a_{ik})g(a_{ik})|\epsilon_{ik}\Omega| = \int_\Omega \bar{V}(x)g(x)\,\mathrm{d}x, \tag{4.8}$$

where

$$\bar{V}(x) := \int_{\mathbb{R}^{n\times n}_{\mathrm{inv}}} v(s)\nu_x(\mathrm{d}s).$$

In view of Lemma 4.9, let us assume that $\{\nu_{a_{ik}}\}_{x\in\Omega} \in \mathcal{GY}^{+\infty,-\infty}(\Omega;\mathbb{R}^{n\times n})$ is a homogeneous gradient Young measure and call $\{\nabla u_j^{ik}\}_{j\in\mathbb{N}}$ its generating sequence. We know that we can consider $\{u_j^{ik}\}_{j\in\mathbb{N}} \subset \mathcal{U}^{\tilde{\varrho}}_{\nabla u(a_{ik})}$ for arbitrary $+\infty > \tilde{\varrho} > \varrho$. Hence

$$\lim_{j\to\infty} \int_\Omega v(\nabla u_j^{ik}(x))g(x)\,\mathrm{d}x = \bar{V}(a_{ik}) \int_\Omega g(x)\,\mathrm{d}x \tag{4.9}$$

and, in addition, u_j^{ik} weakly* converges to the map $x \mapsto \nabla u(a_{ik})x$ for $j \to \infty$ in $W^{1,\infty}(\Omega;\mathbb{R}^n)$.

Let $\Omega_\ell := \{x \in \Omega;\ \mathrm{dist}(x,\partial\Omega) \ge \ell^{-1}\}$. We define a sequence of smooth cut-off functions $\{\eta_\ell\}_{\ell\in\mathbb{N}}$

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

such that $|\nabla\eta_\ell| \le C\ell$ for some $C > 0$. Further, take a sequence $\{u_k^\ell\}_{k,\ell\in\mathbb{N}} \subset W^{1,\infty}(\Omega;\mathbb{R}^n)$ defined by

$$u_k^\ell(x) := \begin{cases} \left[u(a_{ik}) + \epsilon_{ik}u_j^{ik}\left(\frac{x-a_{ik}}{\epsilon_{ik}}\right)\right]\left(1-\eta_\ell\left(\frac{x-a_{ik}}{\epsilon_{ik}}\right)\right) & \\ +u(x)\eta_\ell\left(\frac{x-a_{ik}}{\epsilon_{ik}}\right) & \text{if } x\in a_{ik}+\epsilon_{ik}\Omega, \\ u(x) & \text{otherwise,} \end{cases}$$

where $j = j(i,k,\ell)$ will be chosen later. Note that for every k we have $u_k^\ell - u \in W_0^{1,\infty}(\Omega,\mathbb{R}^n)$.

We calculate for $x \in a_{ik} + \epsilon_{ik}\Omega$

$$\begin{aligned} \nabla u_k^\ell(x) &= \nabla u_j^{ik}\left(\frac{x-a_{ik}}{\epsilon_{ik}}\right)\left(1-\eta_\ell\left(\frac{x-a_{ik}}{\epsilon_{ik}}\right)\right) \\ &\quad + \nabla u(x)\eta_\ell\left(\frac{x-a_{ik}}{\epsilon_{ik}}\right) \\ &\quad + \frac{1}{\epsilon_{ik}}\left[u(x)-u(a_{ik})-\epsilon_{ik}\nabla u(a_{ik})\left(\frac{x-a_{ik}}{\epsilon_{ik}}\right)\right]\otimes\nabla\eta_\ell\left(\frac{x-a_{ik}}{\epsilon_{ik}}\right) \\ &\quad + \left[\nabla u(a_{ik})\left(\frac{x-a_{ik}}{\epsilon_{ik}}\right) - u_j^{ik}\left(\frac{x-a_{ik}}{\epsilon_{ik}}\right)\right]\otimes\nabla\eta_\ell\left(\frac{x-a_{ik}}{\epsilon_{ik}}\right). \end{aligned} \tag{4.10}$$

Notice that the moduli of all four terms can be made together uniformly bounded by $\tilde\varrho > \varrho$. Namely, notice that the sum of the first two terms is not greater then ϱ and the other two terms can be made arbitrarily small if k is sufficiently large compared to ℓ by exploiting (4.6) and the strong convergence in $L^\infty(a_{ik}+\epsilon_{ik}\Omega;\mathbb{R}^n)$ of $u_j^{ik}(x)$ to the map $x \mapsto \nabla u(a_{ik})x$ for $j \to \infty$.

Take the set $(a_{ik}+\varepsilon_{ik}\Omega)\setminus(a_{ik}+\varepsilon_{ik}\Omega_\ell)$ and solve the inclusion $\nabla\tilde u_k^\ell \in O(n)$ with the boundary conditions $\tilde u_k^\ell = u_k^\ell/\tilde\varrho$ if $x \in \partial((a_{ik}+\varepsilon_{ik}\Omega_k)\setminus(a_{ik}+\varepsilon_{ik}\Omega_\ell))$. This inclusion has a solution due to Lemma 4.1. Set

$$z_k^\ell(x) := \begin{cases} u_k^\ell(x) & \text{if } x\in a_{ik}+\epsilon_{ik}\Omega_\ell, \\ \tilde u_k^\ell(x) & \text{if } x\in(a_{ik}+\epsilon_{ik}\Omega)\setminus(a_{ik}+\epsilon_{ik}\Omega_\ell), \\ u(x) & \text{otherwise.} \end{cases}$$

Observe, that the Lebesgue measure of the set $\{x\in\Omega;\ \nabla(u_k^\ell(x)-z_k^\ell(x))\neq 0\}$ vanishes as $\ell\to\infty$. Further, $\{z_k^\ell\}_{k,\ell\in\mathbb{N}} \subset W^{1,\infty}(\Omega;\mathbb{R}^n)$ is a bounded sequence as well as $\{\nabla z_k^\ell\}^{-1}_{k,\ell\in\mathbb{N}} \subset L^\infty(\Omega;\mathbb{R}^{n\times n})$.

Let us fix k, i, ℓ (with k sufficiently large such that $|\nabla z_k^\ell|$ is uniformly bounded by $\tilde\varrho$) and consider the sets $\{E_k\}_{k\in\mathbb{N}}$, $E_k \subset E_{k+1}$ such that $\Gamma\times S = \bigcup_k E_k$. We can eventually enlarge each $j = j(i,k,\ell)$ so that additionally for any $(g, v_0) \in E_k$

$$\left|\epsilon_{ik}^n\int_\Omega g(a_{ik}+\epsilon_{ik}y)v(\nabla u_j^{ik}(y))\,\mathrm{d}y - \bar V(a_{ik})\int_{a_{ik}+\epsilon_{ik}\Omega} g(x)\,\mathrm{d}x\right| \le \frac{1}{2^ik}. \tag{4.11}$$

We have, by the smallness of $|\Omega\setminus\Omega_\ell|$ and boundedness of g and v, that for some $C > 0$

$$\int_\Omega g(x)v(\nabla u_k^\ell(x))\,\mathrm{d}x = \sum_i \epsilon_{ik}^n\int_\Omega g(a_{ik}+\epsilon_{ik}y)v(\nabla u_j^{ik}(y))\,\mathrm{d}y + \frac{C}{\ell}.$$

Consequently, in view of (4.8), (4.7) and (4.11) for all $(g, v) \in \Gamma \times S$

$$\lim_{\ell\to\infty}\lim_{k\to\infty}\int_\Omega g(x)v(\nabla u_k^\ell(x))\,\mathrm{d}x = \int_\Omega\int_{\mathbb{R}^{\times n}} v(s)\nu_x(\mathrm{d}s)g(x)\,\mathrm{d}x.$$

Hence, we can pick a subsequence $\{\nabla u^\ell_{k(\ell)}\}_{\ell\in\mathbb{N}}$ generating ν. The measure ν is also generated by $\{\nabla z^\ell_{k(\ell)}\}_{\ell\in\mathbb{N}}$ because the difference of both sequences vanishes in measure. Finally, we see from the construction that $\{z^\ell_{k(\ell)}\}_{\ell\in\mathbb{N}}$ can be chosen to have the same boundary conditions as u. □

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Chapter 5

Weak lower semicontinuity of integral functional

Jan Krämer, Stefan Krömer, Martin Kružík*, and Gabriel Pathó

$\mathcal{A}$-quasiconvexity at the boundary and weak lower semicontinuity of integral functionals

Abstract: We state necessary and sufficient conditions for weak lower semicontinuity of $u \mapsto \int_\Omega h(x, u(x))\,\mathrm{d}x$ where $|h(x,s)| \le C(1+|s|^p)$ is continuous and possesses a recession function, and $u \in L^p(\Omega;\mathbb{R}^m)$, $p > 1$, lives in the kernel of a constant-rank first-order differential operator $\mathcal{A}$ which admits an extension property. In the special case $\mathcal{A} = \mathrm{curl}$, the recession function's quasiconvexity at the boundary in the sense of J.M. Ball and J. Marsden is known to play a crucial role. Our newly defined notions of $\mathcal{A}$-quasiconvexity at the boundary, generalize this. Moreover, we give an equivalent condition for weak lower semicontinuity of the above functional along sequences weakly converging in $L^p(\Omega;\mathbb{R}^m)$ and approaching the kernel of $\mathcal{A}$ even if $\mathcal{A}$ does not have the extension property.

Keywords: $\mathcal{A}$-quasiconvexity, concentrations, oscillations

MSC: 49J45, 35B05

1 Introduction

In this paper, we investigate the influence of concentration effects generated by sequences $\{u_k\} \subset L^p(\Omega;\mathbb{R}^m)$, $1 < p < +\infty$, which satisfy a linear differential constraint $\mathcal{A}u_k = 0$ ($\mathcal{A}$-free sequence), or $\mathcal{A}u_k \to 0$ in $W^{-1,p}(\Omega;\mathbb{R}^d)$ (asymptotically $\mathcal{A}$-free sequence), on weak lower semicontinuity of integral functionals in the form

$$I(u) := \int_\Omega h(x, u(x))\,\mathrm{d}x\ . \tag{1.1}$$

Here $\mathcal{A}$ is a first-order linear differential operator. To the best of our knowledge, the first such result was proved in [15] for nonnegative integrands. In

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this case, the crucial necessary and sufficient condition ensuring this property is the so-called $\mathcal{A}$-quasiconvexity; cf. Definition 2.5 below. However, if we refrain from considering only nonnegative integrands, this condition is not necessarily sufficient. A prominent example is $\mathcal{A}$=curl, i.e., when u has a potential. It is well known that besides (Morrey's) quasiconvexity weak lower semicontinuity of $I(u) := \int_\Omega h(x, u(x))\,\mathrm{d}x$ for $|h(x, s)| \leq C(1 + |s|^p)$ (i.e. possibly negative and noncoercive) also strongly depends on the behavior of $h(\cdot, s)$ on the boundary of Ω. This was first observed by N. Meyers [24] and then elaborated more explicitly in [20]. Moreover, it turns out that for the special case where $h(x, \cdot)$ possesses a recession function the precise condition is the so-called quasiconvexity at the boundary [3, 22]. Namely, if $\{u_k\} \subset L^p(\Omega; \mathbb{R}^m)$ is a weakly converging sequence, concentrations of $\{|u_k|^p\} \subset L^1(\Omega; \mathbb{R}^m)$ at the boundary of Ω can destroy weak lower semicontinuity. We refer to [6, 13] for general background and [17, 18] for a thorough analysis of oscillation and concentration effects in the gradient (curl-free) case.

The situation is considerably more complicated in case of more general operators $\mathcal{A}$. Some observations can be found in [21], but the focus there is on the behavior of minimizing sequences and in particular, no local conditions on the integrand in the spirit of quasiconvexity at the boundary are derived. In order to see the problem we are facing here, let us isolate a necessary condition for weak lower semicontinuity of I in a simple prototypical situation, a possible candidate to replace quasiconvexity at the boundary for general $\mathcal{A}$.

Example 1.1. Consider a unit half-ball $\Omega := B(x_0, 1) \cap \{x \mid (x - x_0) \cdot \nu_{x_0} \leq 0\} \subset \mathbb{R}^n$, with some fixed unit vector ν_{x_0}. We are mainly interested in the behavior near x_0, where the boundary of Ω is locally flat with normal ν_{x_0} (a boundary of class C^1 actually suffices for the argument below, with some additional technicalities). In addition, we assume for simplicity that the integrand $h : \mathbb{R}^m \to \mathbb{R}$ is smooth and positively p-homogeneous, i.e., for any $\ell \geq 0$ and $s \in \mathbb{R}^m$, $h(\ell s) = \ell^p h(s)$. Given any $u \in L^p(\mathbb{R}^n; \mathbb{R}^m) \cap \ker \mathcal{A}$ such that u is compactly supported in $B(0, 1)$, lower semicontinuity along $\{u_k\} \subset L^p(\mathbb{R}^n; \mathbb{R}^m) \cap \ker \mathcal{A}$, $u_k(x) := k^{n/p} u(k(x - x_0))$, then implies $\liminf_{k\to\infty} I(u_k) \geq I(0) = 0$, because $u_k \rightharpoonup 0$ in L^p. Since $I(u_k) = \int_\Omega h(u)\,\mathrm{d}x$ for all k by a change of variables, shifting x_0 to the origin we get a necessary condition on h: for all $u \in L^p(B(0, 1); \mathbb{R}^m) \cap \ker \mathcal{A}$ such that u vanishes near the boundary of $B(0, 1)$

$$\int_{B(0,1)\cap\{x\cdot\nu_{x_0}\leq 0\}} h(u(x))\,\mathrm{d}x \geq 0 = \int_{B(0,1)\cap\{x\cdot\nu_{x_0}\leq 0\}} h(0)\,\mathrm{d}x \tag{1.2}$$

for all $u \in L^p(B(0, 1); \mathbb{R}^m) \cap \ker \mathcal{A}$ with $u = 0$ near $\partial B(0, 1)$.

It is clear that for the positively p-homogeneous function h, (1.2) generalizes quasiconvexity at the boundary at the zero matrix (for gradients, i.e., curl-free fields) to more general differential constraints given by $\mathcal{A}$. Hence, in case $\mathcal{A}$ =curl and together with quasiconvexity, (1.2) (at every $x_0 \in \partial\Omega$, for a smooth domain Ω) is also sufficient for weak lower semicontinuity. However, as the example below shows, this is no longer true for general $\mathcal{A}$, which also means that (1.2) *is too weak to act as the correct generalization of quasiconvexity at the boundary* for our purposes:

Example 1.2. Let $n = m = 2$, $p = 2$. We take $\mathcal{A}$ to be the differential operator of the Cauchy-Riemann system, i.e., $\mathcal{A}u = 0$ if and only if $\partial_1 u_1 - \partial_2 u_2 = 0 = \partial_2 u_1 + \partial_1 u_2$ (which in turn means that $u_1 + iu_2$ is holomorphic on its domain as a function of $z = x_1 + ix_2 \in \mathbb{C}$). Then (1.2) is trivially satisfied for any function h with $h(0) = 0$, because the only admissible u is the zero function. Similarly, any h is $\mathcal{A}$-quasiconvex: as $\mathcal{A}$-quasiconvexity is tested with periodic functions in $\ker \mathcal{A}$ with zero mean, due to the Liouville theorem the only allowed test function is the zero function. Nevertheless, for $h(x, s) := -|s|^2$ and any bounded domain $\Omega \subset \mathbb{R}^2 \cong \mathbb{C}$ with smooth boundary, I is *not* weakly lower semicontinuous in $L^p \cap \ker \mathcal{A}$: Let $u_k(z) = \frac{1}{k(z-z_k)}$, where $\{z_k\} \subset \mathbb{C} \setminus \Omega$ is a sequence defined in such a way that $\int_\Omega |u_k(x)|^2 \,\mathrm{d}x = 1$ (there always exists such a z_k by continuity, because for fixed k, $\int_\Omega |u_k|^2 \,\mathrm{d}x \to 0$ as $|z_k| \to \infty$ and $\int_\Omega |u_k|^2 \,\mathrm{d}x \to +\infty$ as $\operatorname{dist}(z_k; \Omega) \to 0$). In particular, z_k approaches the boundary of Ω from the outside as k increases. Then $u_k \rightharpoonup 0$ in $L^2(\Omega; \mathbb{R}^2)$ but $\liminf_{k\to\infty} I(u_k) = -1 < I(0) = 0$.

The example shows that test functions in the operator kernel and with zero "boundary conditions" do not suffice to analyze concentration effects on the boundary like that of our holomorphic sequence u_k in the example, where a singularity is approaching the boundary from the outside. Replacing the class of test functions in (1.2) by periodic functions with zero mean as in the definition of $\mathcal{A}$-quasiconvexity does not help either, because (1.2) would still be trivially satisfied in the example, now due to the Liouville theorem. Altogether, we see that the problem of weak lower semicontinuity for a generic $\mathcal{A}$ is considerably more involved, once negative integrands are allowed.

Nevertheless, sequences of functions with smaller and smaller support are certainly natural to test weak lower semicontinuity along "point concentrations". The only question is how that should be reflected in an appropriate stronger version of (1.2). This dilemma is resolved below in Definitions 3.2 and 3.1 by allowing test functions to depart (in a controlled way) from the kernel of $\mathcal{A}$. We show that this approach naturally gives a new necessary and sufficient condition for weak lower semicontinuity of I along asymptotically $\mathcal{A}$-free sequences ($\mathcal{A}u_k \to 0$) called here *strong $\mathcal{A}$-quasiconvexity at the boundary*; cf. Def. 3.2, even for quite rough domains. Obviously, strong $\mathcal{A}$-quasiconvexity at the boundary also suffices for wlsc of I along sequences in the kernel of $\mathcal{A}$. We also derive a necessary and sufficient condition for the latter situation, called *$\mathcal{A}$-quasiconvexity at the boundary*; cf. Def. 3.1. As the name suggests, strong $\mathcal{A}$-quasiconvexity at the boundary implies $\mathcal{A}$-quasiconvexity at the boundary, but in general, these notions are not equivalent as outlined in Section 5, where we also discuss a sufficient condition on the operator $\mathcal{A}$ and the domain ensuring equivalence (Def. 5.1). The picture is therefore more complicated than in the case of nonnegative integrands h, where weak $\mathcal{A}$-quasiconvexity (see Def. 2.5) of $h(x, \cdot)$ is known to be a necessary and sufficient condition for weak lower semicontinuity of I [15, Thm 3.6, 3.7] in both cases, i.e. if $\mathcal{A}u_k = 0$ or if $\mathcal{A}u_k \to 0$ in $W^{-1,p}(\Omega; \mathbb{R}^d)$.

Let us emphasize that variational problems with differential constraints naturally appear in hyperelasticity, electromagnetism, or in micromagnetics [7, 26, 27] and are closely related to the theory of compensated compactness [25, 29, 30]. The concept of $\mathcal{A}$-quasiconvexity goes back to [5] and has been proved to be useful as a unified approach to variational problems with differential constraints, including results on homogenization [4, 11], dimension reduction [19] and characterization of generalized Young measures [2] in the $\mathcal{A}$-free setting. Moreover, first results on $\mathcal{A}$-quasiaffine functions and weak continuity appeared in [16]. As to weak lower semicontinuity, the theory was first developed for nonnegative integrands in [15] as mentioned before, with extensions to nonnegative functionals with nonstandard growth [14] and the case of an operator $\mathcal{A}$ with nonconstant coefficients [28]. The recent work [1] analyzes lower semicontinuity of functionals with linearly growing integrands, including negative integrands but excluding concentrations at the domain boundary.

The plan of the paper is as follows. We first recall some needed definitions and results in Section 2. Our newly derived conditions which, together with $\mathcal{A}$-quasiconvexity precisely characterize weak lower semicontinuity are studied in Section 3. The main results are summarized in Theorem 4.2 and Theorem 4.5. After the concluding remarks in the final section, some auxiliary material is provided in the appendix.

2 Preliminaries

Unless explicitly stated otherwise, we always work with a bounded domain $\Omega \subset \mathbb{R}^n$ such that $\mathcal{L}^n(\partial\Omega) = 0$, equipped with the Euclidean topology and the n-

dimensional Lebesgue measure $\mathcal{L}^n$. $L^p(\Omega,\mathbb{R}^m)$, $1 \le p \le +\infty$, is the standard Lebesgue space. Furthermore, $W^{1,p}(\Omega;\mathbb{R}^m)$, $1 \le p < +\infty$, stands for the usual space of measurable mappings which together with their first (distributional) derivatives are integrable with the p-th power. The subspace of mappings in $W^{1,p}(\Omega;\mathbb{R}^m)$ with zero traces is standardly denoted $W^{1,p}_0(\Omega;\mathbb{R}^m)$. If $1 < p < +\infty$ then $W^{-1,p}(\Omega;\mathbb{R}^m)$ denotes the dual space of $W^{1,p'}_0(\Omega;\mathbb{R}^m)$, where $p'^{-1} + p^{-1} = 1$. A sequence $\{u_k\}$ converges to zero in measure if $\mathcal{L}^n(\{x \in \Omega : |u_k(x)| \ge \delta\}) \to 0$ as $k \to \infty$, for every $\delta > 0$.

We say that $v \in \Upsilon^p(\mathbb{R}^m)$ if there exists a continuous and positively p-homogeneous function $v_\infty : \mathbb{R}^m \to \mathbb{R}$ such that

$$\lim_{|s|\to\infty} \frac{v(s) - v_\infty(s)}{|s|^p} = 0 \ . \tag{2.1}$$

Such a function is called the *recession function* of v. It is well-known that $v/|\cdot|^p$ with $v \in \Upsilon^p(\mathbb{R}^m)$ can be continuously extended on the compactification of $\mathbb{R}^m$ by the sphere, denoted here $\beta_{\mathcal{S}}\mathbb{R}^m$.

2.1 The operator $\mathcal{A}$ and $\mathcal{A}$-quasiconvexity

Following [15], we consider linear operators $A^{(i)} : \mathbb{R}^m \to \mathbb{R}^d$, $i = 1, \dots, n$, and define $\mathcal{A} : L^p(\Omega;\mathbb{R}^m) \to W^{-1,p}(\Omega;\mathbb{R}^d)$ by

$$\mathcal{A}u := \sum_{i=1}^n A^{(i)} \frac{\partial u}{\partial x_i} \ \text{, where} \ \ u : \Omega \to \mathbb{R}^m \ ,$$

i.e., for all $w \in W^{1,p'}_0(\Omega;\mathbb{R}^d)$

$$\langle \mathcal{A}u, w\rangle = -\sum_{i=1}^n \int_\Omega A^{(i)} u(x) \cdot \frac{\partial w(x)}{\partial x_i} \, \mathrm{d}x \ .$$

For $w \in \mathbb{R}^n$ we define the linear map

$$\mathbb{A}(w) := \sum_{i=1}^n w_i A^{(i)} \ : \ \mathbb{R}^m \to \mathbb{R}^d \ .$$

Throughout this article, we assume that there is $r \in \mathbb{N} \cup \{0\}$ such that

$$\text{rank } \mathbb{A}(w) = r \text{ for all } w \in \mathbb{R}^n \ , |w| = 1 \ , \tag{2.2}$$

i.e., $\mathcal{A}$ has the so-called *constant-rank property.*

Below we use $\ker \mathcal{A}$ to denote the set of all locally integrable functions u such that $\mathcal{A}u = 0$ in the sense of distributions, i.e., $\int u \cdot \mathcal{A}^* w \, \mathrm{d}x = 0$ for all $w \in C^\infty$ compactly supported in the domain, where $\mathcal{A}^* = -\sum_{i=1}^n \left(A^{(i)}\right)^T \frac{\partial u}{\partial x_i}$ is the formal adjoint of $\mathcal{A}$. Of course, $\ker \mathcal{A}$ depends on the domain considered, which always should be clear from the context below. In particular, a periodic function u in the space

$$L^p_\#(\mathbb{R}^n;\mathbb{R}^m) := \{u \in L^p_{\mathrm{loc}}(\mathbb{R}^n;\mathbb{R}^m) : \ u \text{ is } Q\text{-periodic}\}$$

is in $\ker \mathcal{A}$ if and only if $\mathcal{A}u = 0$. Here and in the following, Q denotes the unit cube $(-1/2, 1/2)^n$ in $\mathbb{R}^n$, and we say that $u : \mathbb{R}^n \to \mathbb{R}^m$ is *Q-periodic* if for all $x \in \mathbb{R}^n$ and all $z \in \mathbb{Z}^n$

$$u(x + z) = u(x) \ .$$

We will use the following lemmas proved in [15, Lemma 2.14] and [15, Lemma 2.15], respectively.

Lemma 2.1 (projection onto $\mathcal{A}$-free fields in the periodic setting). *There is a linear bounded operator $\mathcal{T} : L^p_\#(\mathbb{R}^n;\mathbb{R}^m) \to L^p_\#(\mathbb{R}^n;\mathbb{R}^m)$ that vanishes on constant functions, $\mathcal{T}(\mathcal{T}u) = \mathcal{T}u$ for all $u \in L^p_\#(\mathbb{R}^n;\mathbb{R}^m)$, and $\mathcal{T}u \in \ker \mathcal{A}$. Moreover, for all $u \in L^p_\#(\mathbb{R}^n;\mathbb{R}^m)$ with $\int_Q u(x)\,\mathrm{d}x = 0$ it holds that*

$$\|u - \mathcal{T}u\|_{L^p_\#(\mathbb{R}^n;\mathbb{R}^m)} \leq C\|\mathcal{A}u\|_{W^{-1,p}_\#(\mathbb{R}^n;\mathbb{R}^d)} \ ,$$

where $C > 0$ is a constant independent of u and $W^{-1,p}_\#$ denotes the dual space of $W^{1,p'}_\#$ ($\frac{1}{p'} + \frac{1}{p} = 1$), the Q-periodic functions in $W^{1,p'}_{loc}(\mathbb{R}^n;\mathbb{R}^m)$ equipped with the norm of $W^{1,p'}(Q;\mathbb{R}^m)$.

Remark 2.2. For every $w \in W^{-1,p}_\#(\mathbb{R}^n)$, we have $\|w\|_{W^{-1,p}(Q)} \leq \|w\|_{W^{-1,p}_\#(\mathbb{R}^n)}$. The converse inequality does not hold, not even up to a constant. However, Lemma 2.1 is often applied to (a sequence of) functions supported in a fixed set $G \subset\subset Q$ (up to periodicity, of course). One can always find a constant $C = C(\Omega, p, G)$ such that

$$\|\mathcal{A}u\|_{W^{-1,p}_\#(\mathbb{R}^n;\mathbb{R}^d)} \leq C\|\mathcal{A}u\|_{W^{-1,p}(Q;\mathbb{R}^d)}$$

for every $u \in L^p(Q;\mathbb{R}^m)$ with $u = 0$ a.e. on $Q \setminus G$.

To achieve this, the Q-periodic test functions used in the definition of the norm in $W^{-1,p}_\#$ can be multiplied with a fixed cut-off function $\eta \in C_0^\infty(Q;[0,1])$ with $\eta = 1$ on G to make them admissible (i.e., elements of $W^{1,p'}_0(Q)$) for the supremum defining the norm in $W^{-1,p}$. This enlarges their norm in $W^{1,p'}$ at most by a constant factor which only depends on p and $\|\nabla\eta\|_{L^\infty(Q)}$ (and thus the distance of G to ∂Q).

Lemma 2.3 (Decomposition Lemma). *Let $\Omega \subset \mathbb{R}^n$ be bounded and open, $1 < p < +\infty$, and let $\{u_k\} \subset L^p(\Omega;\mathbb{R}^m)$ be bounded and such that $\mathcal{A}u_k \to 0$ in $W^{-1,p}(\Omega;\mathbb{R}^d)$ strongly and $u_k \rightharpoonup u$ in $L^p(\Omega;\mathbb{R}^m)$ weakly. Then there is a sequence $\{z_k\} \subset L^p(\Omega;\mathbb{R}^m) \cap \ker \mathcal{A}$ such that $\{|z_k|^p\}$ is equiintegrable in $L^1(\Omega)$ and $u_k - z_k \to 0$ in measure in Ω.*

We also point out the following simple observation made in the proof of Lemma 2.15 in [15], which is useful if we need to truncate $\mathcal{A}$-free or "asymptotically" $\mathcal{A}$-free sequences:

Lemma 2.4. *Let $\Omega \subset \mathbb{R}^n$ be open and bounded, and let $\{u_k\} \subset L^p(\Omega;\mathbb{R}^m)$ be a bounded sequence such that $\mathcal{A}u_k \to 0$ in $W^{-1,p}(\Omega;\mathbb{R}^d)$ strongly and $u_k \rightharpoonup 0$ in $L^p(\Omega;\mathbb{R}^m)$ weakly. Then for every $\eta \in C^\infty(\mathbb{R}^n)$, $\mathcal{A}(\eta u_k) \to 0$ in $W^{-1,p}(\Omega;\mathbb{R}^d)$.*

Proof. $\mathcal{A}(\eta u_k) = \eta \mathcal{A}u_k + \sum_{i=1}^n u_k A^{(i)} \frac{\partial \eta}{\partial x_i} \to 0$ in $W^{-1,p}$, the second term due to the compact embedding of L^p into $W^{-1,p}$. □

Definition 2.5. [see [15, Def. 3.1, 3.2]] We say that a continuous function $v : \mathbb{R}^m \to \mathbb{R}$, $|v| \le C(1 + |\cdot|^p)$ for some $C > 0$, is $\mathcal{A}$-*quasiconvex* if for all $s_0 \in \mathbb{R}^m$ and all $\varphi \in L^p_\#(Q;\mathbb{R}^m) \cap \ker \mathcal{A}$ with $\int_Q \varphi(x)\,\mathrm{d}x = 0$ it holds

$$v(s_0) \le \int_Q v(s_0 + \varphi(x))\,\mathrm{d}x\ .$$

Besides curl-free fields, admissible examples of $\mathcal{A}$-free mappings include solenoidal fields where $\mathcal{A} = \operatorname{div}$ and higher-order gradients where $\mathcal{A}u = 0$ if and only if $u = \nabla^{(\kappa)}\varphi$ for some $\varphi \in W^{\kappa,p}(\Omega;\mathbb{R}^\ell)$, and some $\kappa \in \mathbb{N}$ (for more details see Subsection 5.3, where $\kappa = 2$).

2.2 Weak lower semicontinuity

Let $I : L^p(\Omega;\mathbb{R}^m) \to \mathbb{R}$ be defined as

$$I(u) := \int_\Omega h(x, u(x))\,\mathrm{d}x\ . \tag{2.3}$$

Analogously, we define $I_\infty : L^p(\Omega;\mathbb{R}^m) \to \mathbb{R}$

$$I_\infty(u) := \int_\Omega h_\infty(x, u(x))\,\mathrm{d}x\ , \tag{2.4}$$

where $h_\infty(x,\cdot)$ is the recession function of $h(x,\cdot)$ for $h : \bar{\Omega} \times \mathbb{R}^m \to \mathbb{R}$ continuous such that $h(x,\cdot) \in \Upsilon^p(\mathbb{R}^m)$ for all $x \in \bar{\Omega}$.

Definition 2.6.
(i) We say that a sequence $\{u_k\} \in L^p(\Omega;\mathbb{R}^m)$ is asymptotically $\mathcal{A}$-free if $\|\mathcal{A}u_k\|_{W^{-1,p}(\Omega;\mathbb{R}^m)} \to 0$ as $k \to \infty$.
(ii) A functional I as in (2.3) is called weakly sequentially lower semicontinuous (wslsc) along asymptotically $\mathcal{A}$-free sequences in $L^p(\Omega;\mathbb{R}^m)$ if there is $\liminf_{k\to\infty} I(u_k) \geq I(u)$ for all such sequences that weakly converge to some limit u in L^p.
(iii) Analogously, we say that a functional I is weakly sequentially lower semicontinuous (wslsc) along $\mathcal{A}$-free sequences in $L^p(\Omega;\mathbb{R}^m)$ if

$$\liminf_{k\to\infty} I(u_k) \geq I(u) \text{ for all } \{u_k\} \subset L^p(\Omega;\mathbb{R}^m) \cap \ker \mathcal{A}.$$

We have the following result which was proved in [12, Theorem 2.4] in a slightly less general version. However, its original proof directly extends to this setting.

Theorem 2.7. *Let $h : \bar{\Omega} \times \mathbb{R}^m \to \mathbb{R}$ be continuous such that $h(x,\cdot) \in \Upsilon^p(\mathbb{R}^m)$ for all $x \in \bar{\Omega}$ and $h(x,\cdot)$ is $\mathcal{A}$-quasiconvex for almost every $x \in \Omega$, $1 < p < +\infty$. Then I is sequentially weakly lower semicontinuous in $L^p(\Omega;\mathbb{R}^m) \cap \ker \mathcal{A}$ if and only if*

$$\liminf_{k\to\infty} I_\infty(w_k) \geq I_\infty(0) = 0 \tag{2.5}$$

for every bounded sequence $\{w_k\} \subset L^p(\Omega;\mathbb{R}^m) \cap \ker \mathcal{A}$ with $w_k \to 0$ in measure.

The statement of Theorem 2.7 remains valid if we replace the sequences in $\ker \mathcal{A}$ with asymptotically $\mathcal{A}$-free sequences.

Theorem 2.8. *With h and p as in Theorem 2.7, I is wslsc along asymptotically $\mathcal{A}$-free sequences in $L^p(\Omega;\mathbb{R}^m)$ if and only if (2.5) holds for any bounded, asymptotically $\mathcal{A}$-free sequence $\{w_k\} \subset L^p(\Omega;\mathbb{R}^m)$ such that $w_k \to 0$ in measure.*

Proof. Let $\{u_k\} \subset L^p(\Omega;\mathbb{R}^m)$ be asymptotically $\mathcal{A}$-free and let $\{z_k\}$ and $\{w_k\}$ be defined by the Lemma 2.3. In particular, $\{z_k\} \subset L^p(\Omega;\mathbb{R}^m) \cap \ker \mathcal{A}$. Consider suitable subsequences so that $\liminf = \lim$. Using [12, Formula (A.10)] and the fact that the linear hull of $\{g \otimes v/|\cdot|^p : g \in C(\bar{\Omega}),\, v \in \Upsilon^p(\mathbb{R}^m)\}$ is dense in $C(\bar{\Omega} \times \beta_{\mathcal{S}}\mathbb{R}^m)$ we have

$$\lim_{k\to\infty} \int_\Omega h(x, u_k(x))\,\mathrm{d}x = \lim_{k\to\infty} \int_\Omega h(x, z_k(x))\,\mathrm{d}x + \lim_{k\to\infty} \int_\Omega h_\infty(x, w_k(x))\,\mathrm{d}x\ , \tag{2.6}$$

As $\{|z_k|^p\}$ as well as $\{h(x, z_k(x))\}$ are equiintegrable and $z_k \rightharpoonup u$ we get $\lim_{k\to\infty} I(z_k) \geq I(u)$ in view of [12, Thm. 2.3(i)] (or one can use [15,

Thm. 4.1.]). Thus, $\lim_{k\to\infty} I(u_k) \geq I(u) + \lim_{k\to\infty} I_\infty(w_k)$. This means that $\lim_{k\to\infty} I_\infty(w_k) \geq 0 = I_\infty(0)$ is a sufficient condition for sequential weak lower semicontinuity of I.
On the other hand, assume that $z_k = 0$ for all $k \in \mathbb{N}$, so that $u_k = w_k$ and $u_k \rightharpoonup 0$. Consequently, by (2.6)

$$\lim_{k\to\infty} I(u_k) = I(0) + \lim_{k\to\infty} I_\infty(w_k)$$

and $\lim_{k\to\infty} I(u_k) \geq I(0)$ only if $\lim_{k\to\infty} I_\infty(w_k) \geq 0 = I_\infty(0)$, i.e., this condition is also necessary.

□

Remark 2.9. In fact, since $\mathcal{A}$-quasiconvex effectively prevents negative energy contributions of oscillations, weak lower semicontinuity for such integrands can only fail due to sequences concentrating large values on small sets. Concentrations in the interior cannot play a role either, only sequences $\{u_k\}$ which tend to zero in measure and concentrate at the boundary in the sense that $\{|u_k|^p\}$ converges weakly* to a measure $\sigma \in \mathcal{M}(\bar{\Omega})$ with $\sigma(\partial\Omega) > 0$.

3 Notions of $\mathcal{A}$-quasiconvexity at the boundary

The two conditions introduced below play a crucial role in our characterization of weak lower semicontinuity of integral functionals. They are typically applied to the recession function h_∞ of an integrand h with p-growth.

Before we state them, we fix some additional notation frequently used in what follows:

$$L^p_0(\Omega;\mathbb{R}^m) := \{u \in L^p(\Omega;\mathbb{R}^m);\ \operatorname{supp} u \subset \Omega\},$$
$$C^p_{\text{hom}}(\mathbb{R}^m) := \{v \in C(\mathbb{R}^m);\ v \text{ is positively } p\text{-homogeneous}\}.$$

A norm in C^p_{hom} is given by the supremum norm taken on the unit sphere in $\mathbb{R}^m$. Moreover, whenever a larger domain comes into play, functions in $L^p_0(\Omega;\mathbb{R}^m)$ are understood to be extended by zero to $\mathbb{R}^n \setminus \Omega$ without changing notation.

The definitions given below are stated in a form which is the most natural in the proofs of our main results, and also suitable for rather general domains. For domains with a boundary of class C^1, equivalent, simpler variants more closely resembling the original notion of quasiconvexity at the boundary in the sense of Ball and Marsden are presented in Proposition 3.8–Proposition 3.10.

Definition 3.1. We say that $h_\infty \in C(\bar{\Omega}; C^p_{\text{hom}}(\mathbb{R}^m))$ is $\mathcal{A}$-quasiconvex at the boundary ($\mathcal{A}$-qcb) at $x_0 \in \partial\Omega$ if for every $\varepsilon > 0$ there are $\delta > 0$ and $\alpha > 0$ such that

$$\int_{B(x_0,\delta)\cap\Omega} h_\infty(x, u(x)) + \varepsilon |u(x)|^p \, \mathrm{d}x \geq 0 \tag{3.1}$$

for every $u \in L^p_0(B(x_0, \delta); \mathbb{R}^m)$ with $\|\mathcal{A}u\|_{W^{-1,p}(\mathbb{R}^n;\mathbb{R}^d)} < \alpha \|u\|_{L^p(B(x_0,\delta)\cap\Omega;\mathbb{R}^m)}$.

The next notion is intimately related to weak lower semicontinuity along asymptotically $\mathcal{A}$-free sequences. Notice that the *only but crucial* difference between Definitions 3.1 and 3.2 is the norm used to measure $\mathcal{A}u$.

Definition 3.2. We say that $h_\infty \in C(\bar{\Omega}; C^p_{\text{hom}}(\mathbb{R}^m))$ is strongly $\mathcal{A}$-quasiconvex at the boundary (strongly-$\mathcal{A}$-qcb) at $x_0 \in \partial\Omega$ if for every $\varepsilon > 0$ there are $\delta > 0$ and $\alpha > 0$ such that

$$\int_{B(x_0,\delta)\cap\Omega} h_\infty(x, u(x)) + \varepsilon |u(x)|^p \, \mathrm{d}x \geq 0 \tag{3.2}$$

for every $u \in L^p_0(B(x_0, \delta); \mathbb{R}^m)$ with $\|\mathcal{A}u\|_{W^{-1,p}(\Omega;\mathbb{R}^d)} < \alpha \|u\|_{L^p(B(x_0,\delta)\cap\Omega;\mathbb{R}^m)}$.

As we will show below, strong $\mathcal{A}$-qcb is natural in the characterization for weak lower semicontinuity along asymptotically $\mathcal{A}$-free sequences, while $\mathcal{A}$-qcb plays the same role for weak lower semicontinuity along precisely $\mathcal{A}$-free sequences. While strong $\mathcal{A}$-qcb always implies $\mathcal{A}$-qcb, they are not equivalent in general (see Section 5).

Remark 3.3. Due to the fact that $\mathcal{A}u$ in Definition 3.1 is required to be small on $B(x_0, \delta)$, a set which is not fully contained in Ω, $\mathcal{A}$-qcb as defined above can only be natural if there is an $\mathcal{A}$-free extension operator on $L^p(\Omega; \mathbb{R}^m)$, cf. Definition 4.3 below. However, the existence of such an extension operator may require sufficient smoothness of $\partial\Omega$ and, worse, it strongly depends on $\mathcal{A}$ (it fails for the Cauchy-Riemann system, e.g.). The strong variant of $\mathcal{A}$-qcb does not have this unpleasant implicit dependence on $\mathcal{A}$-free extension properties.

Remark 3.4. In Definition 3.1, $\mathcal{A}u$ is measured in the norm of $W^{-1,p}(\mathbb{R}^n; \mathbb{R}^d)$, but instead of $\mathbb{R}^n$, other domains for this space can be used as well. More precisely, $\mathbb{R}^n$ can be replaced by any domain S_δ compactly containing $B(x_0, \delta)$, because $\mathcal{A}u$ is a distributions supported on $B(x_0, \delta)$. For this class of distributions, the norms of $W^{-1,p}(\mathbb{R}^n; \mathbb{R}^d)$ and $W^{-1,p}(S_\delta; \mathbb{R}^d)$ are equivalent (with constants depending on δ that can be absorbed by α). In particular, $\mathcal{A}$-qcb can also be defined using the class of all $u \in L^p_0(B(x_0, \frac{\delta}{2}); \mathbb{R}^m)$ with

$\|\mathcal{A}u\|_{W^{-1,p}(B(x_0,\delta);\mathbb{R}^d)} < \alpha\|u\|_{L^p(B(x_0,\delta)\cap\Omega;\mathbb{R}^m)}$. Similarly, the class of test functions in Definition 3.2 can be replaced by the set of all $u \in L^p_0(B(x_0,\frac{\delta}{2});\mathbb{R}^m)$ such that $\|\mathcal{A}u\|_{W^{-1,p}(\Omega\cap B(x_0,\delta);\mathbb{R}^d)} < \alpha\|u\|_{L^p(\Omega\cap B(x_0,\delta);\mathbb{R}^m)}$.

Remark 3.5. In Definition 3.1 as well as in Definition 3.2, if for a given $\varepsilon > 0$ the estimate holds for some $\delta > 0$, then it also holds for any $\tilde{\delta} < \delta$ in place of δ, provided that $u \in L^p_0(B(x_0,\tilde{\delta});\mathbb{R}^m)$. Hence, both $\mathcal{A}$-qcb and strong $\mathcal{A}$-qcb are local properties of h_∞ in the x variable, since it suffices to study arbitrarily small neighborhoods of x_0.

It is possible to formulate several equivalent variants of the definitions of $\mathcal{A}$-quasiconvexity at the boundary. In particular, the following proposition shows that the first variable of h can be "frozen" in Definition 3.2.

Proposition 3.6. *A function $(x,s) \mapsto h_\infty(x,s)$, $h_\infty \in C(\bar{\Omega};C^p_{hom}(\mathbb{R}^m))$, is strongly $\mathcal{A}$-qcb at $x_0 \in \partial\Omega$ if and only if $s \mapsto h_\infty(x_0,s)$ is strongly $\mathcal{A}$-qcb at $x_0 \in \partial\Omega$.*

Proof. Let $\varepsilon > 0$ and recall that if (3.1) holds for some $\delta > 0$ then it holds also for any $0 < \tilde{\delta} < \delta$ in the place of δ. We have

$$\begin{aligned} &\left| \int\limits_{B(x_0,\delta)\cap\Omega} \left[h_\infty\left(x, \frac{u(x)}{|u(x)|}\right) - h_\infty\left(x_0, \frac{u(x)}{|u(x)|}\right)\right] |u(x)|^p \,\mathrm{d}x \right| \\ &\quad \leq \int\limits_{B(x_0,\delta)\cap\Omega} \mu(|x-x_0|)|u(x)|^p \,\mathrm{d}x \leq M(\delta) \int\limits_{B(x_0,\delta)\cap\Omega} |u(x)|^p \,\mathrm{d}x \end{aligned} \tag{3.3}$$

where $\mu : \mathbb{R} \to \mathbb{R}$ is a continuous modulus of continuity of the continuous function h_∞ restricted to the compact set $\bar{\Omega} \times S^{m-1}$ and $M(\delta) := \max_{x\in\overline{B(x_0,\delta)\cap\Omega}} \mu(|x-x_0|)$. In particular, $M(\delta) \to 0$ as $\delta \to 0$. Due to (3.3) and the p-homogeneity of h_∞ in its second variable, (3.1) implies that

$$\begin{aligned} &\int\limits_{B(x_0,\delta)\cap\Omega} h_\infty(x_0,u(x)) + (M(\delta)+\varepsilon)|u(x)|^p \,\mathrm{d}x \\ &\qquad\qquad \geq \int\limits_{B(x_0,\delta)\cap\Omega} h_\infty(x,u(x)) + \varepsilon|u(x)|^p \,\mathrm{d}x \geq 0 \;, \end{aligned}$$

whence $(x,s) \mapsto h_\infty(x_0,s)$ is strongly $\mathcal{A}$-qcb at x_0. Here, note that $M(\delta)+\varepsilon$ can be made arbitrarily small if δ is small enough. The converse implication is proved analogously. □

Exactly as in the case of Definition 3.2, the first variable of h_∞ can be "frozen" in Definition 3.1:

Proposition 3.7. *A function $(x,s) \mapsto h_\infty(x,s)$, $h_\infty \in C(\bar{\Omega}; C^p_{hom}(\mathbb{R}^m))$, is $\mathcal{A}$-qcb at $x_0 \in \partial\Omega$ if and only if $(x,s) \mapsto h(x_0,s)$ is $\mathcal{A}$-qcb at $x_0 \in \partial\Omega$.*

By itself, "freezing" the first variable of h does not help to really simplify Definition 3.1 or Definition 3.2, because the possibly complicated local shape of the domain can still prevent passing to the limit as $\delta \to 0$ in a meaningful way. However, this is the best we can do without imposing further restrictions on the smoothness of $\partial\Omega$. Even for Lipschitz domains, the general form of the Definitions typically cannot be avoided (see [20, Remark 1.8] for a more detailed discussion of this in the gradient case corresponding to $\mathcal{A}$=curl).

So far it is not clear to what extent the notion of (strong) $\mathcal{A}$-qcb depends on the local shape of $\partial\Omega$ near the boundary point x_0 under consideration. The propositions below show that at least for domains with smooth boundary we can in some sense pass to the limit as $\delta \to 0$ in Definition 3.1 and Definition 3.2, and the definitions do not depend on any other properties of the domain apart from the outer normal.

Proposition 3.8. *Assume that $\Omega \subset \mathbb{R}^n$ has a C^1-boundary in a neighborhood of $x_0 \in \partial\Omega$. Let ν_{x_0} be the outer unit normal to $\partial\Omega$ at x_0 and*

$$D_{x_0} := \{x \in B(0,1) \mid x \cdot \nu_{x_0} < 0\}.$$

Then $v \in C^p_{hom}(\mathbb{R}^m)$ is strongly-$\mathcal{A}$-qcb at x_0 if and only if

$$\begin{aligned} &\text{for every } \varepsilon > 0 \text{ there exists } \beta > 0 \text{ such that} \\ &\int_{D_{x_0}} v(\varphi(x)) + \varepsilon|\varphi(x)|^p \,\mathrm{d}x \geq 0 \\ &\forall \varphi \in L^p_0(B(0,\tfrac{1}{2}); \mathbb{R}^m)\colon \|\mathcal{A}\varphi\|_{W^{-1,p}(D_{x_0};\mathbb{R}^d)} \leq \beta\|\varphi\|_{L^p(D_{x_0};\mathbb{R}^m)}. \end{aligned} \tag{3.4}$$

Proof. Without loss of generality let us assume $x_0 = 0$. We adapt the proof which appeared already in [20] for the gradient case.

"only if": Suppose that v is strongly-$\mathcal{A}$-qcb at 0. Take $\varepsilon > 0$ and get α, $\delta > 0$ such that

$$\int_{B(0,\delta)\cap\Omega} v(u(x)) + \varepsilon|u(x)|^p \,\mathrm{d}x \geq 0 \tag{3.5}$$

for every $u \in L^p_0(B(0,\frac{\delta}{2}); \mathbb{R}^m)$ such that there is $\|\mathcal{A}u\|_{W^{-1,p}(B(0,\delta)\cap\Omega;\mathbb{R}^d)} \leq \alpha\|u\|_{L^p(B(0,\delta)\cap\Omega;\mathbb{R}^m)}$. Introducing the scaling $\Phi_\delta\colon \overline{B(0,\delta)} \ni x \mapsto \delta^{-1}x \in \overline{B(0,1)}$, the inequality (3.5) can be rewritten as

$$\int_{\delta^{-1}(\Omega\cap B(0,\delta))} v(y(x')) + \varepsilon |y(x')|^p \, dx' \geq 0 \ , \ \text{where } y := \delta^{n/p} u \circ \Phi_\delta^{-1} \tag{3.6}$$

Due to the smoothness of the boundary near zero, there exists a transformation $\Psi_\delta \colon \overline{B(0,1)} \to \overline{B(0,1)}$ such that $\Psi_\delta(0) = 0$, $\Psi_\delta(B(0,\frac{1}{2})) = B(0,\frac{1}{2})$ and $\Psi_\delta(D_0) = \delta^{-1}(\Omega \cap B(0,\delta))$, while both Ψ_δ and its inverse Ψ_δ^{-1} converge to the identity in $C^1(\overline{B(0,1)};\mathbb{R}^n)$ as $\delta \to 0$. We refer to [20, p. 400] or [3, p. 257] for a similar construction. Hence, (3.6) leads to

$$\int_{D_0} (v(\varphi(z)) + \varepsilon|\varphi(z)|^p) |\mathrm{det} \mathrm{D}_z \Psi_\delta(z)| \, dz \geq 0 \ , \tag{3.7}$$

where $\varphi := y \circ \Psi_\delta$ and $[\mathrm{D}_z\Psi_\delta]_{ij} := \partial \Psi_{\delta i}/\partial z_j$ for i, $j = 1, \dots, n$. Due to the boundedness of $v + \varepsilon|\cdot|^p$ and the (uniform) continuity of the transformation Ψ_δ on the unit sphere, we have the estimate

$$|(v(\varphi(z)) + \varepsilon|\varphi(z)|^p)(|\mathrm{det}\mathrm{D}_z\Psi_\delta(z)| - 1)| \leq \varepsilon|\varphi(z)|^p \ , \tag{3.8}$$

for $\delta > 0$ sufficiently small. Incorporating (3.8) into (3.7), we see that

$$\int_{D_0} (v(\varphi(z)) + 2\varepsilon|\varphi(z)|^p) \, dz \geq 0 \ .$$

It remains to find some $\beta = \beta(\varepsilon, \delta, \alpha) > 0$, such that for any admissible φ in (3.4), the associated function $u = \delta^{-\frac{n}{p}} \varphi \circ \Psi_\delta^{-1} \circ \Phi_\delta$ is admissible as a test function in (3.5), i.e., we need that $\|\mathcal{A}\varphi\|_{W^{-1,p}(D_0;\mathbb{R}^d)} \leq \beta\|\varphi\|_{L^p(D_0;\mathbb{R}^m)}$ implies that $\|\mathcal{A}u\|_{W^{-1,p}(B(0,\delta)\cap\Omega;\mathbb{R}^d)} \leq \alpha\|u\|_{L^p(B(0,\delta)\cap\Omega;\mathbb{R}^m)}$.

We calculate

$$\begin{aligned}
&\| \mathcal{A}\varphi \|_{W^{-1,p}(D_0;\mathbb{R}^d)} \\
&\quad = \sup_{\| w \|_{W_0^{1,p'}(D_0;\mathbb{R}^d)} \leq 1} \sum_{i=1}^{n} \int_{D_0} A^{(i)} \varphi(z) \cdot \frac{\partial w(z)}{\partial z_i} \mathrm{d}x \\
&\quad = \sup_{\|w\| \leq 1} \sum_{i=1}^{n} \int_{\Psi_\delta(D_0)} A^{(i)} \varphi(\Psi_\delta^{-1}) \cdot \frac{\partial w}{\partial x_i'}(\Psi_\delta^{-1}(x')) \left|\mathrm{det}\mathrm{D}\Psi_\delta^{-1}(x')\right| \mathrm{d}x' \\
&\quad = \sup_{\|w\| \leq 1} \sum_{i=1}^{n} \int_{\frac{1}{\delta}(B(0,\delta)\cap\Omega)} \sum_{j=1}^{d} \Big(A^{(i)} \varphi(\Psi_\delta^{-1}(x')) \Big)_j \\
&\qquad\qquad \times \Big(\mathrm{D}\big(w(\Psi_\delta^{-1}(x'))\big) \cdot \big(\mathrm{D}\Psi_\delta^{-1}(x')\big)^{-1} \Big)_{j,i} \cdot \mathrm{det}|\mathrm{D}\Psi_\delta^{-1}(\mathrm{x}')|\mathrm{dx}'.
\end{aligned}$$

Denoting $w_\delta := w \circ \Psi_\delta^{-1}$, using the function y as in (3.6) and the convergence of Ψ_δ^{-1} to the identity in $C^1(\overline{B(0,1)};\mathbb{R}^n)$, we get

$$\begin{aligned}
&\| \mathcal{A}\varphi \|_{W^{-1,p}(D_0;\mathbb{R}^d)} \\
&\quad\geq \frac{1}{2} \sup_{\| w_\delta \|_{W_0^{1,p'}(\Psi_\delta(D_0);\mathbb{R}^d)}\leq 1} \sum_{i=1}^n \int_{\frac{1}{\delta}(B(0,\delta)\cap\Omega)} A^{(i)} y(x') \frac{\partial w_\delta(x')}{\partial x_i'} \mathrm{d}x' \\
&\quad= \frac{1}{2} \sup_{\|w_\delta\|\leq 1} \sum_{i=1}^n \int_{B(0,\delta)\cap\Omega} A^{(i)} y(\delta^{-1}x) \frac{\partial w_\delta}{\partial x_i}(\delta^{-1}x)\mathrm{d}x \\
&\quad= \frac{1}{2} \sup_{\|w_\delta\|\leq 1} \sum_{i=1}^n \int_{B(0,\delta)\cap\Omega} A^{(i)} \left(\delta^{n/p} u(x)\right) \delta \frac{\partial(w_\delta(\delta^{-1}x))}{\partial x_i}\mathrm{d}x
\end{aligned}$$

for sufficiently small δ. With $\eta_\delta(x) := \delta^{1-\frac{n}{p'}} w_\delta(\delta^{-1}x)$ and due to

$$\| \mathrm{D}\eta_\delta \|_{L^{p'}(B(0,\delta)\cap\Omega;\mathbb{R}^d)} = \| \mathrm{D}w_\delta \|_{L^{p'}(\frac{1}{\delta}(B(0,\delta)\cap\Omega;\mathbb{R}^d)}$$

it follows that

$$\begin{aligned}
&\| \mathcal{A}\varphi \|_{W^{-1,p}(D_0;\mathbb{R}^d)} \\
&\quad\geq \frac{1}{2} \sup_{\| \eta_\delta \|_{W_0^{1,p'}(B(0,\delta)\cap\Omega;\mathbb{R}^d)}\leq 1} \sum_{i=1}^n \int_{B(0,\delta)\cap\Omega} A^{(i)} u(x) \cdot \frac{\partial \eta_\delta(x)}{\partial x_i} \delta^n \mathrm{d}x \\
&\qquad\qquad= \frac{1}{2}\delta^n \| \mathcal{A}u \|_{W^{-1,p}(B(0,\delta)\cap\Omega;\mathbb{R}^d)}.
\end{aligned}$$

By a similar procedure as above, we compute

$$\begin{aligned}
\|u\|^p_{L^p(B(0,\delta)\cap\Omega;\mathbb{R}^m)} &= \int_{B(0,\delta)\cap\Omega} |u(x)|^p \,\mathrm{d}x \\
&= \int_{\delta^{-1}(B(0,\delta)\cap\Omega)} |u(\Phi_\delta^{-1}(x')|^p |\mathrm{det}\mathrm{D}_{x'}\Phi_\delta^{-1}(x')| \,\mathrm{d}x' = \int_{\delta^{-1}(B(0,\delta)\cap\Omega)} |y(x')|^p \,\mathrm{d}x' \\
&= \int_{D_0} |y(\Psi_\delta(z))|^p |\mathrm{det}\mathrm{D}_z \Psi_\delta(z)| \,\mathrm{d}z \geq \frac{1}{2}\int_{D_0} |\varphi(z)|^p \,\mathrm{d}z = \frac{1}{2}\|\varphi\|^p_{L^p(D_0;\mathbb{R}^m)} .
\end{aligned}$$

In summary,

$$\begin{aligned}
\|\mathcal{A}u\|_{W^{-1,p}(B(0,\delta)\cap\Omega;\mathbb{R}^d)} &\leq 2\delta^{-n}\|\mathcal{A}\varphi\|_{W^{-1,p}(D_0;\mathbb{R}^d)} \\
&\leq 2\delta^{-n}\beta\|\varphi\|_{L^p(D_0;\mathbb{R}^m)} \leq 4\delta^{-n}\beta\|u\|_{L^p(B(0,\delta)\cap\Omega;\mathbb{R}^m)},
\end{aligned}$$

and we therefore choose $\beta = \frac{1}{4}\delta^n\alpha$.

"if": The sufficiency of (3.4) for v to be $\mathcal{A}$-qcb at 0 can be shown by analogous computations, instead of the (uniform) convergence of Ψ_δ one uses the (uniform) convergence of Ψ_δ^{-1} as $\delta \to 0$. □

Following the proof of Proposition 3.8, we are also able to give an equivalent variant of $\mathcal{A}$-qcb in the limit as $\delta \to 0$.

Proposition 3.9. *Assume that $\Omega \subset \mathbb{R}^n$ has a boundary of class C^1 in a neighborhood of $x_0 \in \partial\Omega$. Let ν_{x_0} be the outer unit normal to $\partial\Omega$ at x_0 and*

$$D_{x_0} := \{x \in B(0,1) \mid x \cdot \nu_{x_0} < 0\}.$$

Then $v \in C^p_{hom}(\mathbb{R}^m)$ is $\mathcal{A}$-qcb at x_0 if and only if

$$\begin{aligned} &\text{for every } \varepsilon > 0 \text{ there exists } \beta > 0 \text{ such that} \\ &\int_{D_{x_0}} v(\varphi(x)) + \varepsilon|\varphi(x)|^p \,\mathrm{d}x \geq 0 \\ &\forall \varphi \in L^p_0(B(0,\tfrac{1}{2});\mathbb{R}^m)\colon \|\mathcal{A}\varphi\|_{W^{-1,p}(B(0,1);\mathbb{R}^d)} \leq \beta\|\varphi\|_{L^p(D_{x_0};\mathbb{R}^m)}. \end{aligned} \tag{3.9}$$

Unlike for strong $\mathcal{A}$-qcb, it is possible to derive another version of $\mathcal{A}$-qcb with periodic, precisely $\mathcal{A}$-free test functions and a much more obvious relationship to $\mathcal{A}$-quasiconvexity. Note however that instead of admitting test functions that are only "almost" $\mathcal{A}$-free, we are then forced to work with a class that only "almost" has compact support (since γ can be chosen arbitrarily small in (3.10) below).

Proposition 3.10. *Let $x_0 \in \partial\Omega$, assume that $\partial\Omega$ is of class C^1 in a neighborhood of x_0, and define $Q = Q(x_0) := \{y \in \mathbb{R}^n \mid |y \cdot e_j| < 1 \text{ for } j = 1,\dots,n\}$ and $Q^- := \{y \in Q \mid y \cdot e_1 < 0\}$, where $e_1,\dots,e_n$ of $\mathbb{R}^n$ is an orthonormal basis of $\mathbb{R}^n$ such that $e_1 = \nu_{x_0}$, the unit outer normal to $\partial\Omega$ at x_0. Then $v \in C^p_{hom}(\mathbb{R}^m)$ is $\mathcal{A}$-qcb at x_0 if and only if*

$$\begin{aligned} &\text{for every } \varepsilon > 0, \text{ there exists } \gamma > 0 \text{ such that} \\ &\int_{Q^-} v(\varphi(x)) + \varepsilon|\varphi(x)|^p \,\mathrm{d}x \geq 0 \\ &\forall \varphi \in L^p_\#(Q;\mathbb{R}^m)\colon \mathcal{A}\varphi = 0,\ \|\varphi\|_{L^p(Q\setminus\frac{1}{2}Q;\mathbb{R}^m)} \leq \gamma\|\varphi\|_{L^p(Q;\mathbb{R}^m)}. \end{aligned} \tag{3.10}$$

Proof. "if": We claim that (3.10) implies (3.9). By p-homogeneity, it suffices to show the integral inequality in (3.9) for every $\varphi \in L^p_0(B(0,\frac{1}{2});\mathbb{R}^m)$ with $\|\varphi\|_{L^p} = 1$ and $\|\mathcal{A}\varphi\|_{W^{-1,p}} \leq \beta$, where $\beta = \beta(\varepsilon)$ is yet to be chosen. Below, the average of φ is denoted by

$$a_\varphi := \frac{1}{|Q|} \int\limits_Q \varphi(x)\,\mathrm{d}x.$$

By Lemma 2.1 and Remark 2.2, $\|\varphi - a_\varphi - \mathcal{T}\varphi\|_{L^p(Q;\mathbb{R}^m)}$ becomes arbitrarily small, provided that $\|\mathcal{A}\varphi\|_{W^{-1,p}} \le \beta$ is small enough. In view of Lemma A.3 (uniform continuity of $u \mapsto v(u)$ and $u \mapsto |u|^p$, $L^p \to L^1$, on bounded sets in L^p), this means that for every $\varepsilon > 0$, there exists a $\beta > 0$ such that

$$\int\limits_{Q^-} v(\varphi(x)) + \varepsilon|\varphi(x)|^p\,\mathrm{d}x \ge \int\limits_{Q^-} v(a_\varphi + \mathcal{T}\varphi(x)) + \frac{\varepsilon}{2}|a_\varphi + \mathcal{T}\varphi(x)|^p\,\mathrm{d}x,$$

and due to the inequality in (3.10) with $a_\varphi + \mathcal{T}\varphi$ instead of φ, the right-hand side above is non-negative. Hence,

$$\int\limits_{D_{x_0}} v(\varphi(x)) + \varepsilon|\varphi(x)|^p\,\mathrm{d}x = \int\limits_{Q^-} v(\varphi(x)) + \varepsilon|\varphi(x)|^p\,\mathrm{d}x \ge 0.$$

“only if”: Suppose that (3.9) holds. Let $\varepsilon > 0$, and let φ denote an admissible test function for (3.10), i.e., $\varphi \in L^p_\#(Q_{x_0};\mathbb{R}^m)$ with $\mathcal{A}\varphi = 0$ and $\|\varphi\|_{L^p(Q\setminus\frac{1}{2}Q;\mathbb{R}^m)} \le \gamma\|\varphi\|_{L^p(Q;\mathbb{R}^m)}$, with some γ still to be chosen. We may also assume that $\|\varphi\|_{L^p(Q)} = 1$. Let $\eta \in C_0^\infty(Q;[0,1])$ be a fixed function such that $\eta = 1$ on $\frac{1}{2}Q$ and $\eta = 0$ on $Q \setminus \frac{3}{4}Q$. Observe that $\|\varphi - \eta\varphi\|_{L^p(Q;\mathbb{R}^m)} \le 2\|\varphi\|_{L^p(Q\setminus\frac{1}{2}Q;\mathbb{R}^m)} \le 2\gamma\|\varphi\|_{L^p(Q;\mathbb{R}^m)}$, whence

$$\|\varphi - \eta\varphi\|_{L^p(Q;\mathbb{R}^m)} \le 2\gamma\|\varphi\|_{L^p(Q;\mathbb{R}^m)} \le \frac{2\gamma}{1-2\gamma}\|\eta\varphi\|_{L^p(Q;\mathbb{R}^m)}$$

In addition, there is a constant $C \ge 0$ depending on η and $\mathcal{A}$ such that

$$\begin{aligned}\|\mathcal{A}(\eta\varphi)\|_{W^{-1,p}(Q;\mathbb{R}^d)} &\le C\|\varphi\|_{L^p(\frac{3}{4}Q\setminus\frac{1}{2}Q;\mathbb{R}^m)}\\ &\le C\gamma\|\varphi\|_{L^p(Q;\mathbb{R}^m)} \le \frac{C\gamma}{1-2\gamma}\|\eta\varphi\|_{L^p(Q;\mathbb{R}^m)}.\end{aligned}$$

Hence, for γ sufficiently small, $\eta\varphi$ is an admissible test function for (3.9) (which we apply with $\varepsilon/2$ instead of ε), up to the fact that the support of $\eta\varphi$, which is contained in $\frac{3}{4}Q$, might be larger than $B(0,\frac{1}{2})$. This, however, can be easily corrected by a change of variables, rescaling by a fixed factor. Consequently,

$$\int\limits_{Q^-_{x_0}} v(\eta(x)\varphi(x)) + \frac{\varepsilon}{2}|\eta(x)\varphi(x)|^p\,\mathrm{d}x \ge 0,$$

and due to the uniform continuity shown in Lemma A.3, we conclude that for γ small enough,

$$\int_{Q_{x_0}^-} v(\varphi(x)) + \varepsilon|\varphi(x)|^p \,\mathrm{d}x \geq 0.$$

□

We now focus on the link between (strong) $\mathcal{A}$-quasiconvexity at the boundary and weak lower semicontinuity along (asymptotically) $\mathcal{A}$-free sequences.

4 Link to weak lower semicontinuity

4.1 Asymptotically $\mathcal{A}$-free sequences

Proposition 4.1. *Let $h_\infty \in C(\bar{\Omega}; C^p_{hom}(\mathbb{R}^m))$. Then $I_\infty(u) := \int_\Omega h_\infty(x, u(x))\,\mathrm{d}x$ is weakly sequentially lower semicontinuous along asymptotically $\mathcal{A}$-free sequences in $L^p(\Omega; \mathbb{R}^m)$ if and only if*
(i) h_∞ is strongly-$\mathcal{A}$-qcb at every $x_0 \in \partial\Omega$ and
(ii) $h_\infty(x, \cdot)$ is $\mathcal{A}$-quasiconvex at almost every $x \in \Omega$.

Proof. "only if": We show that strongly-$\mathcal{A}$-qcb at $x_0 \in \partial\Omega$ is a necessary condition; the necessity of (ii) is well known. Suppose that h_∞ is not strongly-$\mathcal{A}$-qcb at $x_0 \in \partial\Omega$. This means that there is $\varepsilon > 0$ such that for every $k \in \mathbb{N}$ there exists $u_k \in L^p_0(B(x_0, \frac{1}{k}); \mathbb{R}^m)$ with $\|\mathcal{A}u\|_{W^{-1,p}(\Omega;\mathbb{R}^d)} \leq \frac{1}{k}\|u_k\|_{L^p(\Omega;\mathbb{R}^m)}$ and

$$\int_{B(x_0,\frac{1}{k})\cap\Omega} h_\infty(x, u_k(x)) + \varepsilon|u_k(x)|^p \,\mathrm{d}x < 0 \ .$$

In particular, u_k cannot be the zero function. Denote

$$\hat{u}_k := u_k/\|u_k\|_{L^p(B(x_0,\frac{1}{k})\cap\Omega;\mathbb{R}^m)} = u_k/\|u_k\|_{L^p(\Omega;\mathbb{R}^m)}.$$

Then $\hat{u}_k \in L^p_0(\Omega; \mathbb{R}^m)$ with $\|\hat{u}_k\|_{L^p} = 1$ and $\|\mathcal{A}\hat{u}_k\|_{W^{-1,p}(\Omega;\mathbb{R}^d)} \leq 1/k$. In addition, $\hat{u}_k$ vanishes outside of $B(x_0, \frac{1}{k})$, so that $\hat{u}_k \to 0$ in measure and weakly in $L^p(B(x_0, 1); \mathbb{R}^m)$. However,

$$\liminf_{k\to\infty} \int_\Omega h_\infty(x, \hat{u}_k(x))\,\mathrm{d}x \leq -\varepsilon < 0 = \int_\Omega h_\infty(x, 0)\,\mathrm{d}x \ .$$

This means that $u \mapsto \int_\Omega h_\infty(x, u(x))\,\mathrm{d}x$ is not lower semicontinuous along $\{\hat{u}_k\}$.

"if": Let us now prove the sufficiency. By Theorem 2.8 and because of (ii), it is enough to show that I_∞ is lower semicontinuous along asymptotically $\mathcal{A}$-free bounded sequences in $L^p(\Omega;\mathbb{R}^m)$ which converge to zero in measure. Let $\{w_k\}$ be such sequence and let $(\pi,\lambda)\in\mathcal{DM}^p_{\mathcal{S}}(\Omega;\mathbb{R}^m)$ be a DiPerna-Majda measure describing $\liminf_{k\to\infty} I_\infty(w_k)$. Take $x_0\in\partial\Omega$ and $\delta>0$ small enough such that $\pi(\partial B(x_0,\delta)\cap\bar{\Omega})=0$. By (A.4)

$$\begin{aligned}\lim_{k\to\infty}\int\limits_{B(x_0,\delta)\cap\Omega} & h_\infty(x,w_k(x))\,\mathrm{d}x\\ &=\int\limits_{\overline{B(x_0,\delta)\cap\Omega}}\ \int\limits_{\beta_{\mathcal{S}}\mathbb{R}^m\setminus\mathbb{R}^m}\frac{h_\infty(x,s)}{1+|s|^p}\mathrm{d}\lambda_x(s)\mathrm{d}\pi(x)\ .\end{aligned} \tag{4.1}$$

Let $\{\eta_\ell\}\subset C_0^\infty(B(x_0,\delta))$ such that $0\le\eta_\ell\le 1$ and $\eta_\ell\to\chi_{B(x_0,\delta)}$ as $\ell\to\infty$. Here, $\chi_{B(x_0,\delta)}$ is the characteristic function of $B(x_0,\delta)$ in $\mathbb{R}^n$ and $x_0\in\partial\Omega$. By Lemma 2.4, $\mathcal{A}(\eta_\ell u_k)\to 0$ in $W^{-1,p}(\Omega;\mathbb{R}^d)$ as $k\to\infty$, for fixed ℓ. Take $\varepsilon>0$, $\alpha,\delta>0$ as in Definition 3.2 and set $\tilde{w}_k:=\eta_{\ell(k)}w_k$, where $\ell(k)$ tends to ∞ sufficiently slowly as $k\to\infty$ so that $\mathcal{A}\tilde{w}_k\to 0$ in $W^{-1,p}(\Omega;\mathbb{R}^d)$. Reasoning as in [12, Appendix], using that $\pi(\partial B(x_0,\delta)\cap\bar{\Omega})=0$, we see that $\{\tilde{w}_k\}$ also generates (π,λ), at least on $\overline{B(x_0,\delta)}\cap\Omega$. If $\tilde{w}_k$ strongly converges to zero in $L^p(\Omega;\mathbb{R}^m)$, we have

$$0=\lim_{k\to\infty}\int\limits_{B(x_0,\delta)\cap\Omega} h_\infty(x,\tilde{w}_k(x))+\varepsilon|\tilde{w}_k(x)|^p\,\mathrm{d}x\ . \tag{4.2}$$

Otherwise, a subsequence of $\{\|\tilde{w}_k\|_{L^p}\}$ (not relabeled) is bounded away from zero, and since $\mathcal{A}\tilde{w}_k\to 0$ in $W^{-1,p}$, this implies that $\|\mathcal{A}\tilde{w}_k\|_{W^{-1,p}}\le\alpha\|\tilde{w}_k\|_{L^p}$, at least for k large enough. Hence, $\tilde{w}_k$ is admissible as a test function in (3.2), and we end up again with (4.2). The right-hand side of (4.2) is nonnegative due to Definition 3.2 and can be expressed using (A.4):

$$\begin{aligned}0\le\lim_{k\to\infty}\int\limits_{B(x_0,\delta)\cap\Omega} & h_\infty(x,\tilde{w}_k(x))+\varepsilon|\tilde{w}_k(x)|^p\,\mathrm{d}x\\ &=\int\limits_{\overline{B(x_0,\delta)\cap\Omega}}\ \int\limits_{\beta_{\mathcal{R}}\mathbb{R}^m\setminus\mathbb{R}^m}\frac{h_\infty(x,s)+\varepsilon|s|^p}{1+|s|^p}\mathrm{d}\lambda_x(s)\mathrm{d}\pi(x)\ .\end{aligned}$$

Hence,

$$0\le\pi(\overline{B(x_0,\delta)\cap\Omega})^{-1}\int\limits_{\overline{B(x_0,\delta)\cap\Omega}}\ \int\limits_{\beta_{\mathcal{R}}\mathbb{R}^m\setminus\mathbb{R}^m}\frac{h_\infty(x,s)+\varepsilon|s|^p}{1+|s|^p}\mathrm{d}\lambda_x(s)\mathrm{d}\pi(x)\ .$$

Therefore, by the Lebesgue-Besicovitch differentiation theorem (see [10], for example) and by taking into account that $\varepsilon > 0$ is arbitrary we get that for π-almost every $x_0 \in \partial\Omega$

$$0 \leq \int\limits_{\beta_{\mathcal{R}}\mathbb{R}^m \setminus \mathbb{R}^m} \frac{h_\infty(x_0, s)}{1+|s|^p} \mathrm{d}\lambda_{x_0}(s) \; .$$

This together with Theorem A.2 and (A.4) implies that the inner integral on the right-hand side of (4.1) is nonnegative for π-almost every $x_0 \in \bar{\Omega}$. As a consequence, I_∞ is lower semicontinuous along $\{u_k\}$. By Theorem 2.8, we conclude that $u \mapsto \int_\Omega h(x, u(x))\, \mathrm{d}x$ is weakly lower semicontinuous along arbitrary asymptotically $\mathcal{A}$-free sequences.

□

In view of Theorem 2.8, our results obtained so far can be summarized as follows.

Theorem 4.2. *Suppose that $\Omega \subset \mathbb{R}^n$ be a bounded domain with $\mathcal{L}^n(\partial\Omega) = 0$. Let $1 < p < +\infty$, and let $h : \bar{\Omega} \times \mathbb{R}^m \to \mathbb{R}$ be continuous and such that $h(x, \cdot) \in \Upsilon^p(\mathbb{R}^m)$ for all $x \in \bar{\Omega}$, with recession function $h_\infty \in C(\overline{\Omega}; C^p_{hom})$. Then I is weakly lower semicontinuous along asymptotically $\mathcal{A}$-free sequences if and only if*
(i) $h(x, \cdot)$ is $\mathcal{A}$-quasiconvex for almost all $x \in \Omega$;
(ii) h_∞ is strongly $\mathcal{A}$-quasiconvex at the boundary for all $x_0 \in \partial\Omega$.

4.2 Genuinely $\mathcal{A}$-free sequences

We now focus on weak lower semicontinuity along sequences $\{u_k\}$ that satisfy $\mathcal{A}u_k = 0$ for each $k \in \mathbb{N}$. Since a substantial part of the arguments in this context is analogous to the ones in the preceding subsection, we do not always give full proofs. The main difference is that for the link to $\mathcal{A}$-quasiconvexity at the boundary ($\mathcal{A}$-qcb) as introduced in Definition 3.1, more precisely, for its sufficiency, we rely on an extension property:

Definition 4.3 ($\mathcal{A}$-free extension domain). We say that Ω is an *$\mathcal{A}$-free extension domain* if there exists a larger domain Ω' with $\Omega \subset\subset \Omega'$ and an associated *$\mathcal{A}$-free extension operator*, i.e., a bounded linear operator $E : L^p(\Omega; \mathbb{R}^m) \cap \ker \mathcal{A} \to L^p(\Omega'; \mathbb{R}^m) \cap \ker \mathcal{A}$ such that $Eu = u$ on Ω.

As mentioned before, the existence of an $\mathcal{A}$-free extension operator not only depends on the smoothness of $\partial\Omega$, but also on $\mathcal{A}$ itself. On the one hand, if $\partial\Omega$ is

Lipschitz, extension operators are available for $\mathcal{A} = \operatorname{curl}$ and $\mathcal{A} = \operatorname{div}$ (essentially using a partition of unity and an extension by a suitable reflection), but on the other hand, if we choose $\mathcal{A}$ to be the differential operator of the Cauchy–Riemann system ($n = m = 2$, identifying $\mathbb{C}$ with $\mathbb{R}^2$), no such extension operator exists even for very smooth domains, since holomorphic functions with singularities at the boundary of Ω can never be extended to holomorphic functions on a larger set including the singular point[1].

With the help of the extension property and the projection $\mathcal{T}$ of Lemma 2.1, Proposition 4.1 can be adapted to the setting of genuinely $\mathcal{A}$-free sequences:

Proposition 4.4. *Suppose that Ω is an $\mathcal{A}$-free extension domain and let $h_\infty \in C(\bar{\Omega}; C^p_{hom}(\mathbb{R}^m))$. Then $I_\infty(u) := \int_\Omega h_\infty(x, u(x))\,\mathrm{d}x$ is weakly sequentially lower semicontinuous along $\mathcal{A}$-free sequences in $L^p(\Omega;\mathbb{R}^m)$ if and only if*
(i) h_∞ is $\mathcal{A}$-qcb at every $x_0 \in \partial\Omega$ and
(ii) $h_\infty(x,\cdot)$ is $\mathcal{A}$-quasiconvex at almost every $x \in \Omega$.

Proof. "only if": Again, necessity of (ii) is well known. If h_∞ is not $\mathcal{A}$-qcb at a point $x_0 \in \partial\Omega$, as in the proof of Proposition 4.1 we obtain an $\varepsilon > 0$ and a sequence $\{\hat{u}_k\} \subset L^p_0(B(x_0, \frac{1}{k}); \mathbb{R}^m)$ with $\|\hat{u}_k\|_{L^p(\Omega;\mathbb{R}^m)} = 1$ such that

$$\liminf_{k\to\infty} \int_\Omega h_\infty(x, \hat{u}_k(x))\,\mathrm{d}x \le -\varepsilon < 0 = \int_\Omega h_\infty(x, 0)\,\mathrm{d}x,$$

and $\|\mathcal{A}\hat{u}_k\|_{W^{-1,p}(\mathbb{R}^n;\mathbb{R}^d)} \le 1/k$. Each $\hat{u}_k$ can be interpreted as a Q-periodic function $\hat{u}^\#_k$ with respect to a cube Q compactly containing $\Omega \cup B(x_0, 1)$, by first extending $\hat{u}_k$ by zero to the rest of Q and then periodically to $\mathbb{R}^n$. We denote its cell average by

$$a_k := \frac{1}{|Q|} \int_Q \hat{u}_k\,\mathrm{d}x.$$

By Remark 2.2, we infer that $\|\mathcal{A}\hat{u}^\#_k\|_{W^{-1,p}_\#(\mathbb{R}^n;\mathbb{R}^d)} \le C/k$ with a constant $C \ge 0$ independent of k. The projection of Lemma 2.1 now yields the sequence $\{\mathcal{T}\hat{u}^\#_k\} \subset L^p_\#(R^n; \mathbb{R}^m) \cap \ker \mathcal{A}$, which satisfies $\|a_k + \mathcal{T}\hat{u}^\#_k - \hat{u}_k\|_{L^p(Q;\mathbb{R}^m)} \to 0$ as $k \to \infty$. Consequently, $a_k + \mathcal{T}\hat{u}^\#_k \rightharpoonup 0$ weakly in L^p just like $\hat{u}_k$, and due to

1 In terms of integrability, the weakest possible point singularity of an elsewhere holomorphic function locally behaves like $z \mapsto 1/z$ ($z \in \mathbb{C}\setminus\{0\}$), which is not in $L^p(\Omega)$ if $p \ge 2$, $0 \in \partial\Omega$ and $\partial\Omega$ is smooth in a neighborhood, but using an appropriately weighted series of singular terms, each with a singularity slightly outside Ω, accumulating at a boundary point, examples in L^p are possible for arbitrary $1 \le p < \infty$.

Lemma A.3 (uniform continuity on bounded subsets of L^p),

$$\liminf_{k\to\infty} \int_\Omega h_\infty(x, a_k + \mathcal{T}\hat{u}_k^{\#}(x))\,\mathrm{d}x \le -\varepsilon < 0 = \int_\Omega h_\infty(x,0)\,\mathrm{d}x.$$

Hence, I_∞ is not lower semicontinuous along the $\mathcal{A}$-free sequence $\{a_k + \mathcal{T}\hat{u}_k^{\#}\}$.
“if”: The argument is completely analogous to that of Proposition 4.1, using Theorem 2.7 instead of Theorem 2.8. Observe that due to the extension operator, any given sequence $\{u_k\}$ along which we want to show lower semicontinuity is defined and $\mathcal{A}$-free on some set $\Omega' \supset\supset \Omega$. Hence, after the truncation argument of Proposition 4.1, we now end up with an admissible test function for Definition 3.1 (see also Remark 3.4). □

We arrive at the analogous main result:

Theorem 4.5. *Suppose that $\Omega \subset \mathbb{R}^n$ be a bounded $\mathcal{A}$-free extension domain with $\mathcal{L}^n(\partial\Omega) = 0$. Let $1 < p < +\infty$, and let $h : \bar{\Omega} \times \mathbb{R}^m \to \mathbb{R}$ be continuous and such that $h(x,\cdot) \in \Upsilon^p(\mathbb{R}^m)$ for all $x \in \bar{\Omega}$, with recession function $h_\infty \in C(\overline{\Omega}; C^p_{hom})$. Then I is sequentially weakly lower semicontinuous along $\mathcal{A}$-free sequences if and only if*
(i) $h(x,\cdot)$ is $\mathcal{A}$-quasiconvex for almost all $x \in \Omega$;
(ii) h_∞ is $\mathcal{A}$-quasiconvex at the boundary for all $x_0 \in \partial\Omega$.

Remark 4.6. In general, the continuity of h_∞ in x cannot be dropped in Theorem 4.5. For a counterexample in the gradient case ($\mathcal{A}$ =curl) see [20, Section 4].

5 Concluding remarks

5.1 $\mathcal{A}$-free versus asymptotically $\mathcal{A}$-free sequences

It is obvious that weak lower semicontinuity along asymptotically $\mathcal{A}$-free sequences implies weak sequential lower semicontinuity for the functional restricted to $\ker \mathcal{A}$. We do not know whether or not the converse is true in general. However, it holds at least in some special cases. More precisely, it suffices to have an extension property in the following sense. It trivially implies the $\mathcal{A}$-free extension property mentioned in Definition 4.3 (but the converse is not clear there, either):

Definition 5.1 (asymptotically $\mathcal{A}$-free extensions). We say that Ω has the $\mathcal{A}$-(L^p,$W^{-1,p}$) extension property if there exists a domain Λ with $\bar{\Omega} \subset\subset \Lambda$ and a linear operator $E : L^p(\Omega;\mathbb{R}^m) \to L^p(\Lambda;\mathbb{R}^m)$ such that for every $u \in L^p(\Omega;\mathbb{R}^m)$, $Eu = u$ on Ω,

$$\|Eu\|_{L^p(\Lambda;\mathbb{R}^m)} \leq C\|u\|_{L^p(\Omega;\mathbb{R}^m)} \text{ and } \|\mathcal{A}Eu\|_{W^{-1,p}(\Lambda;\mathbb{R}^d)} \leq C\|\mathcal{A}u\|_{W^{-1,p}(\Omega;\mathbb{R}^d)},$$

where $C \geq 0$ is a suitable constant.

If this holds, we can always reduce asymptotically $\mathcal{A}$-free sequences to genuinely $\mathcal{A}$-free sequences with arbitrarily small error in L^p. The argument can be sketched as follows: For a given approximately $\mathcal{A}$-free sequence $u_k \rightharpoonup u$ along which we want to show lower semicontinuity, it is possible to truncate the extension of $u_k - u$, multiplying with a cut-off function which is 1 on Ω and makes a transition down to zero in $\Lambda \setminus \Omega$ (this cannot be done inside, because u_k might concentrate a lot of mass near the boundary, and cutting off inside could then significantly alter the limit of the functional along the sequence). The modified sequence is still asymptotically $\mathcal{A}$-free due to Lemma 2.4, and since it is compactly supported in Λ by construction, we can further extend it periodically to $\mathbb{R}^n$, with a sufficiently large fundamental cell of periodicity containing the support of the cut-off function. We thus end up in the periodic setting where we can project onto $\mathcal{A}$-free fields with controllable error, using Lemma 2.1.

Clearly, the $\mathcal{A}$-(L^p,$W^{-1,p}$) extension property implies the standard $\mathcal{A}$-free extension property introduced in Def 4.3, and if the former holds, then $\mathcal{A}$-quasiconvexity at the boundary and strong $\mathcal{A}$-quasiconvexity at the boundary are equivalent. Even for smooth domains, the $\mathcal{A}$-(L^p,$W^{-1,p}$) extension property depends on $\mathcal{A}$ (and possibly on p). For instance, it holds for $\mathcal{A} = \operatorname{div}$ on domains of class C^1 using local maps and extension by an appropriate reflection for flat pieces of the boundary, but not for all $\mathcal{A}$. In particular, it fails for the Cauchy-Riemann system, just like the weaker $\mathcal{A}$-free extension property introduced in Def 4.3. Interestingly, the case $\mathcal{A}$ =curl seems to be nontrivial: the $\mathcal{A}$-(L^p,$W^{-1,p}$) extension property for $\mathcal{A}$ =curl does hold for $n = 2$ (the $2d$-curl and the $2d$-divergence are the same operators up to a fixed rotation), but if $n \geq 3$, we do not know. For a flat piece of the boundary, the natural extension for almost curl-free fields would of course also be by reflection, i.e., the one corresponding to an even extension of the scalar potential across the boundary (even in direction of the normal), but in this case the required estimate in $W^{-1,p}$ for the curl seems to be nontrivial, if true at all. The problem appears for those components of the curl that contain only partial derivatives in the tangential directions, precisely the ones that "naturally" get extended to even functions, say, $\partial_2 u_3 - \partial_3 u_2$, if the normal to the boundary (locally) is the first unit vector.

The situation for smooth domains is summarized in the table below:

$\mathcal{A}$	strong $\mathcal{A}$-qcb $\Leftrightarrow$ $\mathcal{A}$-qcb	Extension property of Def. 5.1
div ($n \in \mathbb{N}$)	**true**	**true**
Cauchy-Riemann ($n = 2$)	**false**	**false**
curl ($n = 2$)	**true**	**true**
curl ($n > 2$)	**open**	**open**

Although the second and the third column in the table coincide we do not know whether the existence of the extension in the sense of Def. 5.1 is really equivalent to $\mathcal{A}$-qcb $\Rightarrow$ strong $\mathcal{A}$-qcb. In view of the constant rank condition (2.2) which makes it hard to characterize the class of the admissible operators $\mathcal{A}$ beyond a few examples, a systematic analysis for all $\mathcal{A}$ seems to be out of reach.

5.2 The gradient case and classical quasiconvexity at the boundary

If $\varphi \in \ker \mathcal{A}$ then (3.4) as well as (3.9) implies that $\int_{D_{x_0}} v(\varphi(x))\, \mathrm{d}x \geq 0$. For $\mathcal{A} = \operatorname{curl}$, the differential constraint can also be encoded using potentials: If $\varphi \in L^p$ and $\operatorname{curl} \varphi = 0$ on the simply connected domain D_{x_0}, then there exists a potential vector field $\Phi \in W^{1,p}$ with $\varphi = \nabla \Phi$, and if $\varphi = 0$ on $D_{x_0} \setminus B(0, \frac{1}{2})$, then Φ inherits this property up to an appropriate choice of the constants of integration. Hence, we get that

$$\int_{D_{x_0}} v(\nabla \Phi(x))\, \mathrm{d}x \geq 0 \qquad \text{for every } \Phi \in W_0^{1,p}(B(0, \tfrac{1}{2}); \mathbb{R}^m). \tag{5.1}$$

Taking into account that for p-homogeneous v, $v(0) = 0$ and $\mathrm{D}v(0) = 0$, the latter condition is the so-called quasiconvexity at the boundary [3] (at the zero matrix).

The converse, that is, going back from (5.1) to either (3.4) or (3.9), is not so obvious, however, because (5.1) does not admit test fields with small but non-zero curl. Nevertheless, in case of (3.9) and for quasiconvex v, this is true as a consequence of known characterizations of weak lower semicontinuity, on the one hand our Proposition 4.4 and the other hand Theorem 1.6 in [20]. (A proof directly working with (5.1) and (3.9), projection and error estimates is also possible, although slightly more technical.)

5.3 Examples for the case of higher order derivatives

The following example shows that $I(u) := \int_\Omega \det \nabla^2 u(x)\,\mathrm{d}x$ is not weakly lower semicontinuous on $W^{2,2}(\Omega)$. Consequently, the determinant is not $\mathcal{A}$-qcb for suitably defined $\mathcal{A}$. As to the definition of $\mathcal{A}$, we recall [15]: The functional I fits into our framework, if instead of $\nabla^2 u$, we define I on fields $v = (v)_{ij}$, $1 \le i \le j \le n$, in L^2, satisfying $\mathcal{A}v := \operatorname{curl}\ v = 0$, with the understanding that for each x, $v(x)$ (the upper triangular part of a matrix) is identified with a symmetric matrix in $\mathbb{R}^{n\times n}$ still denoted v, both for the application of the (row-wise) curl and the evaluation of I, where $\nabla^2 u$ is replaced by v. One can check that $\mathcal{A}v = 0$ if and only if there exists a scalar-valued $u \in W^{2,2}$ with $v = \nabla^2 u$, at least as long as the domain is simply connected.

Example 5.2. Consider $\Omega := (-1,1)^2$ and for $F \in \mathbb{R}^{2\times 2}$ the function $v_\infty(F) := \det F$ and the operator $\mathcal{A}$ such that $\mathcal{A}w = 0$ if and only if for some $u \in W^{2,2}(\Omega)$, w is the upper (or lower) triangular part of $\nabla^2 u$, which takes values in the symmetric matrices; cf. [15, Example 3.10(d)]. Here $\nabla^2 u$ denotes the Hessian matrix of u. Then v_∞ is not $\mathcal{A}$-qcb. Indeed, take $u \in W_0^{2,2}(\Omega)$ extended by zero to the whole $\mathbb{R}^2$. Define $u_k(x) := k^{-1}u(kx)$. Then $u_k \rightharpoonup 0$ in $W^{2,2}(\Omega)$. We have that

$$\lim_{k\to\infty} \int\limits_{(0,1)\times(-1,1)} \det \nabla^2 u_k(x)\,\mathrm{d}x = \int\limits_{(0,1)\times(-1,1)} \det \nabla^2 u(y)\,\mathrm{d}y\ . \tag{5.2}$$

Hence, it remains to find u for which the integral on the right-hand side is negative which is certainly possible.

In the next example, we isolate a function which is $\mathcal{A}$-quasiconvex at the boundary.

Example 5.3. Consider $\Omega := B(0,1) \subset \mathbb{R}^3$ and $\mathcal{A}$ such that $\mathcal{A}w = 0$ if and only if $w = \nabla^2 u$ for some $u \in W^{2,2}(\Omega)$, and the mapping $h(x,F) := a(x)\cdot(\mathrm{Cof}F)\nu(x)$, where $a \in C(\bar{\Omega};\mathbb{R}^3)$ is arbitrary and $\nu(x) \in C(\bar{\Omega})$ coincides with the outer unit normal to $\partial\Omega$ for $x \in \partial\Omega$. Notice that by definition of the Cofactor matrix $((\mathrm{Cof}F)_{ij}$ is $(-1)^{i+j}$ times the determinant of the 2×2 submatrix of F obtained by erasing the i-th row and j-th column), $(\mathrm{Cof}\nabla u(x))\nu(x)$ effectively only depends on directional derivatives of u in directions perpendicular to $\nu(x)$.

For this h,

$$\int\limits_\Omega h(x,\nabla^2 u_k(x))\,\mathrm{d}x \to \int\limits_\Omega h(x,\nabla^2 u_0(x))\,\mathrm{d}x$$

whenever $u_k \rightharpoonup u_0$ in $W^{2,2}(\Omega)$.

To see that consider $z_k := \nabla u_k$ for $k \in \mathbb{N} \cup \{0\}$. Then $\{z_k\} \in W^{1,2}(\Omega; \mathbb{R}^3)$ and the result follows from [17].

A Appendix

A.1 DiPerna-Majda measures

DiPerna-Majda measures are generalizations of Young measures; see [13, 23, 26, 27] for their modern treatment and applications. In what follows, $\mathcal{M}(\bar{\Omega})$ denotes the space of Radon measures on $\bar{\Omega}$. Let $\mathcal{R}$ be a complete (i.e. containing constants, separating points from closed subsets and closed with respect to the supremum norm), separable (i.e. containing a dense countable subset) ring of continuous bounded functions from $\mathbb{R}^m$ into $\mathbb{R}$. It is known that there is a one-to-one correspondence $\mathcal{R} \mapsto \beta_{\mathcal{R}}\mathbb{R}^m$ between such rings and (metrizable) compactifications $\beta_{\mathcal{R}}\mathbb{R}^m$ of $\mathbb{R}^m$ [9]. We only need the special case $\mathcal{R} = \mathcal{S}$ with

$$\mathcal{S} := \left\{ v_0 \in C(\mathbb{R}^m) \,\middle|\, \exists c \in \mathbb{R}\ ,\ v_{0,0} \in C_0(\mathbb{R}^m),\ v_{0,1} \in C(S^{m-1}) \text{ s.t.} \right. \\ \left. v_0(s) = c + v_{0,0}(s) + v_{0,1}\left(\frac{s}{|s|}\right)\frac{|s|^p}{1+|s|^p} \text{ if } s \neq 0 \text{ and } v_0(0) = c + v_{0,0}(0) \right\}, \tag{A.1}$$

where S^{m-1} denotes the $(m-1)$-dimensional unit sphere in $\mathbb{R}^m$. In this case, $\beta_{\mathcal{S}}\mathbb{R}^m$ is obtained by adding a sphere to $\mathbb{R}^m$ at infinity. More precisely, $\beta_{\mathcal{S}}\mathbb{R}^m$ is homeomorphic to the closed unit ball $\overline{B(0,1)} \subset \mathbb{R}^m$ via the mapping $f : \mathbb{R}^m \to B(0,1)$, $f(s) := s/(1+|s|)$ for all $s \in \mathbb{R}^m$. Note that $f(\mathbb{R}^m)$ is dense in $\overline{B(0,1)}$. For simplicity, we will not distinguish between $\mathbb{R}^m$ and its image in $\beta_{\mathcal{S}}\mathbb{R}^m$.

DiPerna and Majda [8] proved the following theorem:

Theorem A.1. *Let Ω be an open domain in $\mathbb{R}^n$ with $\mathcal{L}^n(\partial\Omega) = 0$, and let $\{y_k\} \subset L^p(\Omega; \mathbb{R}^m)$, with $1 \le p < +\infty$, be bounded. Then there exists a subsequence (not relabeled), a positive Radon measure $\pi \in \mathcal{M}(\bar{\Omega})$ and a family of probability measures on $\beta_{\mathcal{S}}\mathbb{R}^m$ $\lambda := \{\lambda_x\}_{x\in\bar{\Omega}}$ such that for all $h_0 \in C(\bar{\Omega} \times \beta_{\mathcal{S}}\mathbb{R}^m)$ it holds that*

$$\lim_{k\to\infty} \int_\Omega h_0(x, y_k(x))(1 + |y_k(x)|^p)dx = \int_{\bar{\Omega}} \int_{\beta_{\mathcal{S}}\mathbb{R}^m} h_0(x,s)d\lambda_x(s)d\pi(x)\ . \tag{A.2}$$

If (A.2) holds we say that $\{y_k\}$ generates (π, λ) and we denote the set of all such pairs of measures generated by some sequence in $L^p(\Omega; \mathbb{R}^m)$ by $\mathcal{DM}^p_{\mathcal{S}}(\Omega; \mathbb{R}^m)$.

For any $h(x,s) := h_0(x,s)(1+|s|^p)$ with $h_0 \in C(\bar{\Omega} \times \beta_{\mathcal{S}}\mathbb{R}^m)$ there exists a continuous and positively p-homogeneous function $h_\infty : \bar{\Omega} \times \mathbb{R}^m \to \mathbb{R}$, i.e., $h_\infty(x,ts) = t^p h_\infty(x,s)$ for all $t \geq 0$, all $x \in \bar{\Omega}$, and $s \in \mathbb{R}^m$, such that

$$\lim_{|s|\to\infty} \frac{h(x,s) - h_\infty(x,s)}{|s|^p} = 0 \quad \text{for all } x \in \bar{\Omega}. \tag{A.3}$$

It is already mentioned in [12, Formula (A.13)] that if $\{y_k\} \subset L^p(\Omega;\mathbb{R}^m)$ is bounded and $\mathcal{L}^n(\{x \in \Omega;\ y_k(x) \neq 0\}) \to 0$ as $k \to \infty$ then it is enough to test (A.2) with recession functions only, i.e., is then equivalent to

$$\lim_{k\to\infty} \int_\Omega h_\infty(x, y_k(x))dx = \int_{\bar{\Omega}} \int_{\beta_{\mathcal{S}}\mathbb{R}^m \setminus \mathbb{R}^m} \frac{h_\infty(x,s)}{1+|s|^p} d\lambda_x(s) d\pi(x) \ , \tag{A.4}$$

where $(x,s) \mapsto h_0(x,s) := h_\infty(x,s)/(1+|s|^p)$ belongs to $C(\bar{\Omega} \times \beta_{\mathcal{S}}\mathbb{R}^m)$ which is the closure (in the maximum norm) of the linear hull of $\{g \otimes v/|\cdot|^p : g \in C(\bar{\Omega}),\ v \in \Upsilon^p(\mathbb{R}^m)\}$.

The following theorem is a direct consequence of [12, Thm. 2.2].

Theorem A.2. *Let $h \in C(\bar{\Omega}; C^p_{hom}(\mathbb{R}^m))$ such that $h(x,\cdot)$ is $\mathcal{A}$-quasiconvex for all $x \in \bar{\Omega}$ (whence h coincides with its $\mathcal{A}$-quasiconvex envelope $Q_{\mathcal{A}}h$, and in particular, $Q_{\mathcal{A}}h(0) = h(0) = 0$), and suppose that $\{y_k\} \subset L^p(\Omega;\mathbb{R}^m) \cap \ker \mathcal{A}$ generates $(\pi,\lambda) \in \mathcal{DM}^p_{\mathcal{S}}(\Omega;\mathbb{R}^m)$. Then for π-almost every $x \in \Omega$,*

$$0 \leq \int_{\beta_{\mathcal{S}}\mathbb{R}^m \setminus \mathbb{R}^m} \frac{h(x,s)}{1+|s|^p} \mathrm{d}\lambda_x(s) \ . \tag{A.5}$$

A.2 Uniform continuity properties of the functional

The following lemma essentially allows us to modify sequences inside I as long as the modified sequences approaches the original one in the norm of L^p.

Lemma A.3. *Let $h_\infty \in C(\bar{\Omega}; C^p_{hom}(\mathbb{R}^m))$. Then for any pair $\{u_k\}$, $\{v_k\}$ of bounded sequences in $L^p(\Omega;\mathbb{R}^m)$ such that $u_k - v_k \to 0$ strongly in L^p, $h_\infty(\cdot, u_k(\cdot)) - h_\infty(\cdot, v_k(\cdot)) \to 0$ strongly in L^1.*

Proof. For $\delta > 0$ let

$$A_k(\delta) := \{x \in \Omega : |u_k(x) - v_k(x)| \geq \delta(|u_k(x)| + |v_k(x)| + 1)\}.$$

Since $u_k - v_k \to 0$ in L^p, we see that

$$\int_{A_k(\delta)} (|u_k(x)| + |v_k(x)| + 1)^p \,\mathrm{d}x \to 0 \text{ as } k \to \infty, \text{ for every } \delta. \tag{A.6}$$

In addition, h_∞ is uniformly continuous on the compact set $\overline{\Omega} \times \overline{B(0,1)} \subset \mathbb{R}^n \times \mathbb{R}^m$, with a modulus of continuity μ, whence

$$\begin{aligned}
&\int\limits_{\Omega\setminus A_k(\delta)} |h_\infty(x,u_k) - h_\infty(x,v_k)|\,\mathrm{d}x \\
&= \int\limits_{\Omega\setminus A_k(\delta)} \bigg| h_\infty\Big(x, \frac{u_k}{|u_k|+|v_k|+1}\Big) \\
&\qquad - h_\infty\Big(x, \frac{v_k}{|u_k|+|v_k|+1}\Big)\bigg| (|u_k(x)|+|v_k(x)|+1)^p\,\mathrm{d}x \\
&\le \int\limits_{\Omega\setminus A_k(\delta)} \mu(\delta)(|u_k(x)|+|v_k(x)|+1)^p\,\mathrm{d}x \\
&\le \mu(\delta)C \underset{\delta\to 0}{\longrightarrow} 0 \quad \text{uniformly in } k,
\end{aligned} \tag{A.7}$$

where we also used that $\{u_k\}$ and $\{v_k\}$ are bounded in L^p. Combining (A.6) and (A.7), $\|h_\infty(\cdot,u_k(\cdot)) - h_\infty(\cdot,v_k(\cdot))\|_{L^1}$ can be made arbitrarily small, first choosing δ small enough and then k large, depending on δ. □

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