Chapter 1
Modeling of thin martensitic films with nonpolynomial stored energies

Martin Kružík and Johannes Zimmer

Abstract A study of the thin film limit of martensitic materials is presented, with the film height tending to zero. The behaviour of the material is modeled by a stored elastic energy which grows to infinity if the normal to the deformed film tends to zero. We show that the macroscopic behavior of the material can be described by gradient Young measures if Dirichlet boundary conditions are prescribed at the boundary of the film. In this situation, we also formulate a rate-independent problem describing evolution of the material. A second approach, perhaps useful in case of non-Dirichlet loading, is presented as well, relying on suitable generalized Young measures.

1.1 Introduction

In this article, we consider the thin film limit of a model for shape-memory alloys. Shape-memory alloys have been the focus of many investigations in the last decade. This interest can partially be attributed to the shape-memory effect itself (see Subsection 1.1.1), but even more the nonconvexity of the Helmholtz energy density due to the co-existence of several variants, which poses a significant mathematical challenge.

Here, our motivation is to address one typical difficulty of modelling shape memory alloys. Namely, a common framework for such models is three-dimensional elasticity, and more specifically hyperelasticity, which means that the first Piola-Kirchhoff stress tensor has a potential W. Static equilibria are minimisers of the elastic energy; one is thus led to solve

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

where $\Omega \subset \mathbb{R}^n$ denotes the reference configuration of the material, ∇ the is gradient operator, $y \in W^{1,p}(\Omega;\mathbb{R}^n)$ is the deformation, with $1 < p < +\infty$, $y = y_0$ on $\partial\Omega$, and $W\colon \mathbb{R}^{n\times n} \to \mathbb{R}$ is the stored energy density.

A central point of interest of this paper is to incorporate the important physical assumption

$$W(F) \to +\infty \text{ whenever } \det(F) \searrow 0 \tag{1.2}$$

(this is related to the physical constraint that an elastic deformation of a body has to be orientation-preserving, which means $\det(\nabla y(x)) > 0$ almost everywhere).

One class of materials where this constraint can be included is that of *polyconvex* W, i.e., $W(F)$ can be written as a convex function of all minors of F. The existence of minimisers to (1.1) was proved by J. M. Ball in his pioneering

M. Kružík
Institute of Information Theory and Automation of the ASCR, Pod vodárenskou věží 4, 182 08 Prague, Czech Republic, and Czech Technical University, Faculty of Civil Engineering, Thákurova 7, 166 29 Prague, Czech Republic

J. Zimmer
Department of Mathematical Sciences, University of Bath, Bath BA2 7AY, United Kingdom

paper [Bal77]. The existence theory for polyconvex energy densities can deal with the growth behaviour (1.2). We refer, e.g., to [Cia88, Dac89] for various results in this direction.

However, materials cannot be modelled by polyconvex stored energies. Prominent examples are materials with microstructure, such as shape-memory materials [BJ87, Mül99], and we see this analysis as a prototype of modelling materials whose stored energy is not polyconvex (or quasiconvex, see below). We develop a framework in which the constraint (1.2) can be included, even in the presence of oscillations and concentrations of minimising functions. Other than the theory for polyconvex functions, there are few results. For a limit leading to a one-dimensional equation (where it is not a significant constraint to be a gradient), Freddi and Paroni develop a comprehensive Young measure approach [FP04], building on earlier work by Acerbi, Buttazzo and Percivale [ABP91]. The requirement (1.2) also appears in the relaxation result by Ben Belgacem [BB00], which is also inspired by [ABP91]. For the full vectorial case, we refer to recent results in this direction by one of the authors and coworkers [BKP11]. Here, we pursue a different line of thought, by considering a thin-film equivalent of (1.2) (see (1.10) below). We exploit the fact that the related quasiconvex envelope has polynomial growth; this allows us to study both the static case and a rate-independent evolution.

1.1.1 Shape memory alloys

Some materials can, after a deformation, recover their original shape upon heating, and this is called the shape memory effect. We summarise key properties of this effect here; see [KZ11] for a more extensive discussion. It is based on the ability of the shape-memory alloy to rearrange atoms in different crystallographic configurations (in particular, with different symmetry groups). Such materials have a high-temperature phase called austenite and a low-temperature phase called martensite. Since austenite is more symmetric, the martensitic phase exists in several variants, with the number of variants M, say, being the quotient of the order of the austenitic symmetry group and the order of the martensitic group. So for a cubic high-symmetry phase, $M = 3$, 6, 12, or 4 for the tetragonal, orthorhombic, monoclinic, respectively triclinic martensites. We denote the stress-free strains of the variants U_ℓ, $\ell = 1,2,\dots,M$, and U_0 stands for the stress-free strain of the austenite. Since the martensitic phase exists in several symmetry related variants, it can form a microstructure by mixing those variants (possibly also with the austenitic variant) on a fine scale. Examples of these coherent combinations are twins of two variants, which is often called a laminate. This ability to form microstructures is one reason why shape memory alloys, as for example Ni-Ti, Cu-Al-Ni or In-Th, have various technological applications.

1.1.2 Variational models for shape memory alloys

Variational models for microstructures assume that formed structure has some optimality property. The reason for the formation of microstructures is that no exact optimum can be achieved and optimising sequences have to develop finer and finer oscillations. A typical example is a microstructure in a shape memory alloy.

We confine ourselves to the case of negligible hysteretic behaviour. This leads to a multidimensional vectorial variational problem, whose relaxation (i.e., suitable extension) is not yet satisfactorily understood. We study microstructures on mesoscopical level, which means that we do not only take care of some macroscopic effective response of the material but also provide some information on optimising sequences. In the last decade, similar mesoscopical models equipped with suitable dissipative potentials have been developed to treat materials with significant hysteresis; see [KMR05, MR03]. For a review of various mathematical problems related to martensitic crystals, we refer the reader to [Mül99].

For shape memory alloys, W is not quasiconvex [Mor08]. We recall that quasiconvexity means that for all $\varphi \in W_0^{1,\infty}(\Omega;\mathbb{R}^n)$ and all $F \in \mathbb{R}^{n\times n}$

$$|\Omega|\,W(F) \le \int_\Omega W(F+\nabla\varphi(x))\,\mathrm{d}x\,; \tag{1.3}$$

we introduce for later use the notation $Qv\colon \mathbb{R}^{m\times n} \to \mathbb{R}$ for the quasiconvex envelope of $v\colon \mathbb{R}^{m\times n} \to \mathbb{R}$. That is,

$$Qv(F)\,|\Omega| := \inf_{\varphi\in W_0^{1,\infty}(\Omega;\mathbb{R}^m)} \int_\Omega v(F+\nabla\varphi(x))\,\mathrm{d}x \,.$$

For energies which are not quasiconvex, minimisers to J in (1.1) do not necessarily exist. However, if we give up (1.2) and suppose that W has polynomial growth at infinity, so that for $c, C > 0$

$$c\,(-1+|F|^p) \le W(F) \le C\,(1+|F|^p)\ , \tag{1.4}$$

the existence of a solution to (1.1) is guaranteed if W is quasiconvex. Here and below, $|F| := \sqrt{\mathrm{tr}(F^\top F)}$ denotes the Frobenius norm of the matrix F.

Yet, quasiconvexity is a complicated property and difficult to verify in most concrete cases. Moreover, as mentioned above, the stored energy densities of materials with microstructure are not quasiconvex. As a result, solutions to (1.1) might not exist. Various relaxation techniques were developed [Dac89, Mül99, Rou97] to overcome this drawback. One is to extend the notion of solutions from Sobolev mappings to parametrised measures called Young measures [Bal89, Rou97, Val94, Tay97]. The idea is to describe limit behaviour of $\{J(y_k)\}_{k\in\mathbb{N}}$ along a minimising sequence $\{y_k\}_{k\in\mathbb{N}}$. Nevertheless, the *growth condition* (1.4) *is still a key ingredient* in these considerations. We sketch in this article a new approach to deal with more general growth conditions, allowing to incorporate (1.2).

1.2 Thin films

1.2.1 Static problems

Bhattacharya and James [BJ99] considered the following problem of a thin film limit. Let $\omega \subset \mathbb{R}^2$ be an open, bounded domain with Lipschitz boundary. We write $I := (0,1)$ and define $\Omega_\varepsilon := \omega \times \varepsilon I$ as the reference state for the space occupied by a specimen. Let $\{e_1, e_2, e_3\}$ be an orthonormal basis in $\mathbb{R}^3$; we suppose that e_3 is perpendicular to the plane of the film, whereas e_1, e_2 lie in the film plane.

The plane gradient $\nabla_{1,2}$ of a (weakly differentiable) map $y : \omega \to \mathbb{R}^3$ denoting deformation is defined as

$$\nabla_{1,2}y = y_{,1}\otimes e_1 + y_{,2}\otimes e_2\ ,$$

where $y_{,i}$ denotes the vector of derivatives of y with respect to x_i, $i = 1,2$. Moreover, having a matrix $F \in \mathbb{R}^{3\times 3}$, we write $F := (f_1|f_2|f_3)$ if $F = f_1\otimes e_1 + f_2\otimes e_2 + f_3\otimes e_3$, where $f_i \in \mathbb{R}^3$ for $i = 1,2,3$.

Bhattacharya and James study the problem

$$\text{minimise } J^\kappa_\varepsilon(y) = \frac{1}{\varepsilon}\int_{\Omega_\varepsilon}\left[W(\nabla y(x)) + \kappa\left|\nabla^2 y(x)\right|^2\right]\mathrm{d}x\ , \tag{1.5}$$

where $\kappa > 0$ is a constant describing the surface energy and

$$y \in \{u \in W^{2,2}(\Omega_\varepsilon;\mathbb{R}^3)\ \big|\ y(x) = Ax \text{ if } x \in \partial\Omega_\varepsilon\}\ ,$$

with $A \in \mathbb{R}^{3\times 3}$ fixed. It is shown that (up to a subsequence), minimisers y^ε, say, of J^κ_ε satisfy for $\varepsilon \to 0$

$$\begin{aligned}
&\nabla^2_{1,2}y^\varepsilon \to \nabla^2_{1,2}\bar{y} \text{ in } L^2(\Omega_1)\ ,\\
&\frac{1}{\varepsilon}\nabla y^\varepsilon_{,3} \to \nabla_{,3}\bar{b} \text{ in } L^2(\Omega_1)\ ,\\
&\frac{1}{\varepsilon^2}y^\varepsilon_{,33} \to 0 \text{ in } L^2(\Omega_1)\ .
\end{aligned}$$

Moreover, $(\bar{y},\bar{b}) \in W^{2,2}(\omega;\mathbb{R}^3)\times W^{1,2}(\omega;\mathbb{R}^3)$ minimise the energy

$$J_0^{\kappa}(y,b) := \int_{\omega}\left[W\left(y_{,1}(x)|y_{,2}(x)|b(x)\right)+\kappa\left(\left|\nabla^2_{1,2}y(x)\right|^2+|\nabla_{1,2}b|^2\right)\right]\,\mathrm{d}S \tag{1.6}$$

subject to the boundary conditions $y(x_1,x_2)=(a_1|a_2)x$ and $b(x_1,x_2)=a_3$ if $(x_1,x_2)\in\partial\omega$. The coefficients $(a_1|a_2|a_3)\in\mathbb{R}^{3\times3}$ are fixed. Physically, $y\colon\,\omega\to\mathbb{R}^3$ describes the the average deformation of the film, while $b\colon\,\omega\to\mathbb{R}^3$ describes the shear of the cross-section of the film. Since κ is small, we may consider the model without the surface energy, i.e., the elastic energy stored in the film is now

$$J_0(y,b) := \int_{\omega} W\left(y_{,1}(x)|y_{,2}(x)|b(x)\right)\,\mathrm{d}S\ . \tag{1.7}$$

The functional $\bar{J}_0$ is nonconvex and minimiser does not have to exists in the set $W^{1,2}(\omega;\mathbb{R}^3)\times L^2(\omega;\mathbb{R}^3)$ equipped with affine boundary conditions.

There is a central difference to the analogous model for the bulk material. Namely, let us consider the situation where $\omega=\omega_1\cup\omega_2\cup L$, with ω_1 and ω_2 being disjoint subsets of ω, and L being a line interface between them, and that

$$(y_{,1}|y_{,2}|b)=\begin{cases}R_iF_i & \text{in } \omega_1\\ R_jF_j & \text{in } \omega_2\ ,\end{cases}$$

where $R_i,R_j\in\mathrm{SO}(3)$ and F_i,F_j are zero energy deformation gradients. One further requires that y is continuous in ω, while $y_{,1}$, $y_{,2}$ as well as b may suffer jumps across the interface L. It is shown in [BJ99] that in order to satisfy these requirements, the following *thin-film twinning equation* must be satisfied

$$R_iF_i-R_jF_j=a\otimes n+c\otimes e_3\ , \tag{1.8}$$

where $a,n\in\mathbb{R}^3$, $n\cdot e_3=0$ and $c\in\mathbb{R}^3$ denotes the jump of b across the interface. The vector n is normal to the line interface. Thus, we say that martensitic variants i and j can form a *linear thin-film interface* if there are rotations R_i,R_j and vectors a,n,c as above that (1.8) holds. We note that this condition is much weaker than the bulk situation, where $\mathrm{rank}(R_iF_i-R_jF_j)=1$ has to hold. Namely, it is a necessary and sufficient condition that one can construct a piecewise affine but continuous map whose gradient only takes values R_iF_i and R_jF_j, $i\neq j$. As a consequence, there are interfaces between martensitic variants in the thin film which cannot exist in the bulk material.

Since the surface energy of the film is not considered here, the model includes only b, but not its gradient. Therefore we can eliminate b from the theory by setting

$$\bar{W}(f_1|f_2) := \min_{b\in\mathbb{R}^3} W(f_1|f_2|b)\ . \tag{1.9}$$

The continuity, coercivity an boundedness of W in the form of (1.4) ensure that a minimum exists. Hence, we can rewrite (1.7) as

$$J(y) := \int_{\omega}\bar{W}\left(y_{,1}(x)|y_{,2}(x)\right)\,\mathrm{d}S\ ,$$

because then the minima of J and J_0 are the same.

If we want to include a condition analogous to (1.2) in the thin-film model, we immediately see that f_1,f_2 in (1.9) should not be parallel, since otherwise $\det(|f_1|f_2|b)=0$. Namely, $f_1\times f_2$ is the normal vector to the thin-film surface in the deformed configuration $y(\omega)$ and $|f_1\times f_2|$ measures area changes. More precisely, if $y\colon\,\omega\to\mathbb{R}^3$ is invertible, then for $O\subset\omega$ measurable

$$\mathrm{meas}(y(O))=\int_O |y_{,1}\times y_{,2}|\,\mathrm{d}S\ .$$

Thus, taking $r>1$, we define the following modified thin-film energy density $\hat{W}\colon\,\mathbb{R}^{3\times2}\to\mathbb{R}\cup\{+\infty\}$

$$\hat{W}(f_1|f_2) := \bar{W}(f_1|f_2)+\frac{1}{|f_1\times f_2|^r}\ . \tag{1.10}$$

Consider $y_0\colon \bar{\omega} \to \mathbb{R}^3$, a continuous and piecewise affine affine mapping, and set

$$W^{1,p}_{y_0}(\omega;\mathbb{R}^3) := \{z \in W^{1,p}(\omega;\mathbb{R}^3);\ z = y_0 \text{ on } \partial\omega\}\ .$$

Moreover, let us define $I\colon W^{1,p}_{y_0}(\omega;\mathbb{R}^3) \to \mathbb{R}\cup\{+\infty\}$,

$$I(y) := \int_\omega \hat{W}\left(y_{,1}(x)|y_{,2}(x)\right)\,\mathrm{d}S$$

and $I_Q\colon W^{1,p}_{y_0}(\omega;\mathbb{R}^3) \to \mathbb{R}\cup\{+\infty\}$,

$$I_Q(y) := \int_\omega Q\hat{W}\left(y_{,1}(x)|y_{,2}(x)\right)\,\mathrm{d}S\ .$$

We immediately see that $\hat{W}$ does not satisfy polynomial growth assumptions and standard coercivity conditions. Nevertheless, we have the following relaxation result due to Anza Hafsa and Mandallena [AHM08, Th. 1.2].

Proposition 1. *Assume that* (1.10) *holds, and let* $+\infty > p > 1$. *Then* $\inf\{I(u);\, u \in W^{1,p}_{y_0}(\omega;\mathbb{R}^3)\} = \min\{I_Q(u);\ u \in W^{1,p}_{y_0}(\omega;\mathbb{R}^3)\}$. *Moreover, if* $\{u_k\} \subset W^{1,p}_{y_0}(\omega;\mathbb{R}^3)$ *is a minimising sequence for I and $u_k \rightharpoonup u$ in* $W^{1,p}(\omega;\mathbb{R}^3)$, *then u is a minimiser to I_Q. On the other hand, if* $\bar{u} \in W^{1,p}_{y_0}(\omega;\mathbb{R}^3)$ *is a minimiser to I_Q, then there is a a minimising sequence* $\{\bar{u}_k\} \subset W^{1,p}_{y_0}(\omega;\mathbb{R}^3)$ *of I which weakly converges to $\bar{u}$ in* $W^{1,p}(\omega;\mathbb{R}^3)$.

The proof of the proposition relies on the fact that $Q\hat{W}$ has a polynomial growth at infinity, i.e., for all $F \in \mathbb{R}^{3\times 2}$, $\left|Q\hat{W}(F)\right| \le C(1+|F|^p)$, with some $C > 0$.

In general, it is not possible to determine the quasiconvex envelope in closed form. There is, however, its representation in terms of gradient Young measures. While finding such a representation is an equally difficult problem, there are known subsets and supsets of gradient Young measures which can be exploited efficiently in numerical calculations [BK11, Kru98].

Let us denote by $\mathscr{G}^{p,r}_{y_0}(\omega;\mathbb{R}^{3\times 2})$ the set of gradient Young measures $\mu = \{\mu_x\}_{x\in\omega}$ generated by sequences of gradients of mappings from $W^{1,p}_{y_0}(\omega;\mathbb{R}^3)\}$ such that for $F = (f_1|f_2) \in \mathbb{R}^{3\times 2}$,

$$\int_\omega \int_{\mathbb{R}^{3\times 2}} (|F|^p + |f_1 \times f_2|^{-r})\mu_x(\mathrm{d}F)\,\mathrm{d}x < +\infty\ .$$

Then we can define the integral functional $\mathscr{J} : \mathscr{G}^{p,r}(\omega;\mathbb{R}^{3\times 2}) \to \mathbb{R}$ as

$$\mathscr{J}(\nu) = \int_\omega \int_{\mathbb{R}^{3\times 2}} \hat{W}(F)\nu_x(\mathrm{d}F)\,\mathrm{d}x\ .$$

Proposition 2. *Let* (1.10) *hold and let $p > 1$ be finite. Then*

$$\min\{I_Q(u);\ u \in W^{1,p}_{y_0}(\omega;\mathbb{R}^3)\} = \inf\{I(u);\ u \in W^{1,p}_{y_0}(\omega;\mathbb{R}^3)\} = \min\{\mathscr{J}(\mu);\ \mu \in \mathscr{G}^{p,r}_{y_0}(\omega;\mathbb{R}^{3\times 2})\}\ .$$

Moreover, if ν minimises $\mathscr{J}$ and $\nabla u(x) = \int_{\mathbb{R}^{3\times 2}} \hat{F}\nu_x(\mathrm{d}F)$ *for almost all $x \in \omega$ and some* $u \in W^{1,p}_{y_0}(\omega;\mathbb{R}^3)$, *then u minimises I_Q. On the other hand, if* $y \in W^{1,p}_{y_0}(\omega;\mathbb{R}^3)$ *minimises I_Q and* $Q\hat{W}(\nabla y(x)) = \int_{\mathbb{R}^{3\times 2}} \hat{W}(F)\mu_x(\mathrm{d}F)$ *for some* $\mu \in \mathscr{G}^{p,r}_{y_0}(\omega;\mathbb{R}^{3\times 2})$, *then μ minimises $\mathscr{J}$.*

Proof. We use the fact that if $\{y_k\} \subset L^p(\Omega;\mathbb{R}^{m\times n})$ and ν is the associated Young measure, then for every normal integrand $\psi\colon \Omega \times \mathbb{R}^{m\times n} \to (-\infty;\infty]$ bounded from below it holds that [FL07, Theorem 8.2]

$$\liminf_{k\to\infty} \int_\Omega \psi(x, y_k(x))\,\mathrm{d}x \ge \int_\Omega \int_{\mathbb{R}^{m\times n}} \psi(x,s)\nu_x(\mathrm{d}s)\,\mathrm{d}x\ . \tag{1.11}$$

The first equality in the proposition then follows from Proposition 1. Indeed, combining Proposition 1 with (1.11), we obtain for a minimising sequence $\{u_k\} \subset W^{1,p}_{y_0}(\omega;\mathbb{R}^3)$ of I converging weakly to u, a minimiser of I_Q, and generating a Young measure ν such that

$$\int_\Omega Q\hat{W}(\nabla u(x))\,\mathrm{d}x = \lim_{k\to\infty} I(u_k) \geq \int_\omega \int_{\mathbb{R}^{3\times 2}} \hat{W}(F)\nu_x(\mathrm{d}F)\,\mathrm{d}x\,. \tag{1.12}$$

At the same time, $\nabla u(x) = \int_{\mathbb{R}^{3\times 2}} F \nu_x(\mathrm{d}F)$ for almost all $x \in \Omega$ and [KP94]

$$Q\hat{W}(\nabla u(x)) \leq \int_{\mathbb{R}^{3\times 2}} Q\hat{W}(F)\nu_x(\mathrm{d}F)\,\mathrm{d}x \leq \int_{\mathbb{R}^{3\times 2}} \hat{W}(F)\nu_x(\mathrm{d}F)\,. \tag{1.13}$$

By combining (1.12) and (1.13), we get that for almost all $x \in \Omega$

$$Q\hat{W}(\nabla u(x)) = \int_{\mathbb{R}^{3\times 2}} \hat{W}(F)\nu_x(\mathrm{d}F) \tag{1.14}$$

and that ν_x is supported on the set $\{F \in \mathbb{R}^{3\times 2};\ Q\hat{W}(F) = \hat{W}(F)\}$ for a.a. $x \in \Omega$. Thus we showed that $\min I_Q \geq \inf \mathscr{J}$. Assume that there is $\mu \in \mathscr{G}^{p,r}_{y_0}(\omega;\mathbb{R}^{3\times 2})$ such that $\mathscr{J}(\mu) < \min I_Q$. Then there is $\{y_k\} \in W^{1,p}_{y_0}(\omega;\mathbb{R}^3)$ such that $\{\nabla y_k\}$ generates μ and $y_k \rightharpoonup y$. Since $\hat{W} \geq Q\hat{W}$, it follows that

$$\begin{aligned}\lim_{k\to\infty} I(y_k) \geq \mathscr{J}(\mu) = \int_\omega \int_{\mathbb{R}^{3\times 2}} \hat{W}(F)\mu_x(\mathrm{d}F) &\geq \int_\omega \int_{\mathbb{R}^{3\times 2}} Q\hat{W}(F)\mu_x(\mathrm{d}F) \\ &\geq \int_\omega Q\hat{W}(\nabla y(x))\,\mathrm{d}x \geq \min I_Q\,,\end{aligned} \tag{1.15}$$

hence $\mathscr{J}(\mu) \geq \min I_Q$ in contradiction to our assumption that $\mathscr{J}(\mu) < \min I_Q$. The second but last inequality in (1.15) follows from Jensen's inequality (for quasiconvex functions, as in the characterisation of gradient Young measures given by Kinderlehrer and Pedregal [KP94]) since $\left|Q\hat{W}(F)\right| \leq C(1+|F|^p)$, as proved in [AHM08]. $\square$

1.2.2 Evolutionary problems

Changes of external conditions typically lead to evolution of material deformation and may initiate phase transformations. This phenomenon is usually connected with energy dissipation. Hence, we enrich our static relaxed model, i.e., the one defined on Young measures ν by a suitable dissipation mechanism and time dependent loading via Dirichlet boundary conditions.

1.2.2.1 Dissipation related to phase transitions

The dissipation mechanism we describe to model phase transition is a two-dimensional version of a common one, for example described in [KZ11]. For completeness, we give a summary, following the presentation in [KZ11]. In order to describe dissipation due to transformations we adopt, as, e.g., [MR03], the standpoint that the amount of dissipated energy associated with a particular phase transition between austenite and a martensitic variant or between two martensitic variants can be described by a specific energy (of the dimension J/m^2). For an explicit definition of the transformation dissipation, we need to identify the particular phases or phase variants. To do so, we define a continuous mapping $\mathscr{L}\colon \mathbb{R}^{3\times 2} \to \triangle$, where

$$\triangle := \Big\{\zeta \in \mathbb{R}^{1+M} \;\Big|\; \zeta_\ell \geq 0 \text{ for } \ell = 1,\ldots,M+1, \text{ and } \sum_{\ell=1}^{M+1} \zeta_\ell = 1\Big\}$$

is a simplex with $M+1$ vertices, with M being the number of martensitic variants. Here $\mathscr{L}$ is related with the material itself and thus has to be frame indifferent. We assume, beside $\zeta_\ell \geq 0$ and $\sum_{\ell=1}^{M+1} \zeta_\ell = 1$, that the coordinate ζ_ℓ of $\mathscr{L}(F)$ takes the value 1 if there is $b \in \mathbb{R}^3$ such that $(F|b)$ is in the ℓth (phase) variant, that is, $(F|b)$ is in a vicinity of the

ℓth well $\mathrm{SO}(n)U_\ell$ of W, which can be identified by the stretch tensor $(F|b)^\top(F|b)$ being close to $U_\ell^\top U_\ell$. Here, $U_\ell^\top U_\ell$ denotes the right Cauchy-Green strain tensors of the stress-free strain states. They represent particular martensitic variants and the austenite. If $\mathscr{L}(F)$ is not in any vertex of $\triangle$, then it means that F is in the spinodal region where no definite phase or variant is specified. We assume, however, that the wells are sufficiently deep and the phases and variants are geometrically sufficiently far from each other that the tendency for minimisation of the stored energy will essentially prevent F to range into the spinodal region. Thus, the concrete form of $\mathscr{L}$ is not important as long as $\mathscr{L}$ enjoys the properties listed above. We remark that $\mathscr{L}$ plays the rôle of what is often called a vector of *order parameters* or a vector-valued *internal variable*.

For two states q_1 and q_2, with $q_j = (y_j, \nu_j, \lambda_j)$ (deformation, Young measure, and volume fraction) for $j = 1,2$, we now define the dissipation due to martensitic transformation which "measures" changes in the volume fraction $\lambda \in L^\infty\left(\Omega;\mathbb{R}^{M+1}\right)$. Although λ_j is given by ν_j, it is convenient to consider them here as a pair of independent variables and put their relationship as a constraint to the set of admissible states. This dissipation is given by

$$\mathscr{D}(q_1,q_2) := \int_\omega |\lambda_1(x) - \lambda_2(x)|_{\mathbb{R}^{M+1}} \mathrm{d}x\,, \tag{1.16}$$

where

$$\lambda_j(x) := \int_{\mathbb{R}^{3\times 2}} \mathscr{L}(F)\nu_{j,x}(\mathrm{d}F) \tag{1.17}$$

and $|\cdot|_{\mathbb{R}^{M+1}}$ is a norm on $\mathbb{R}^{M+1}$. As $\lambda^j(x)$ represents the volume fraction of the jth phase in the material point x we inevitably get $\sum_{j=1}^{M+1}\lambda^j = 1$ and we call λ the vector-valued volume fraction as it gives us relative portions of variants at almost every $x \in \Omega$. In what follows, we will assume that the norm on $\mathbb{R}^{M+1}$ defining the dissipation in (1.16) is given as

$$|X|_{\mathbb{R}^{M+1}} := \sum_{i=1}^{M+1} c^i\left|X^i\right|\,,\ X = (X^1,\ldots,X^{M+1}) \tag{1.18}$$

where $|\cdot|$ is the absolute value and $c^i > 0$ for all i. The physical meaning of c^i is the specific energy dissipated if X^i changes from zero to one (or vice versa).

1.2.2.2 Energetic solution

Combining the previous considerations, we arrive at the energy functional $\mathscr{I}$ of the form

$$\mathscr{I}(t,q) := \int_\omega \int_{\mathbb{R}^{3\times 2}} \hat{W}(F+\nabla y_0(t,x))\nu_x(\mathrm{d}F)\mathrm{d}x + \varepsilon\,\|\nabla\lambda\|_{L^2\left(\omega;\mathbb{R}^{(1+M)\times 2}\right)}\,, \tag{1.19}$$

where the term $\nabla\lambda$ is included to regularise the problem. It penalises spatial jumps of the volume fraction λ and introduces a length scale to the problem, depending on the parameter $\varepsilon > 0$. In particular, it allows us to pass to the limit in the dissipation term. In order to define an admissible set where we look for a solution triple $q = (y,\nu,\lambda)$, we put

$$y \in W^{1,p}_{y_0}(\omega;\mathbb{R}^3) \tag{1.20}$$

Here $y_0(t) \in W^{1,p}(\omega;\mathbb{R}^3)$ with piecewise affine boundary conditions and $t \in [0;\mathfrak{T}]$ ranges within the process time interval, with $\mathfrak{T} > 0$ being the final time.

Then we look for $q \in \mathscr{Q} := W^{1,p}(\omega;\mathbb{R}^m) \times \mathscr{G}_0^{p,r}\left(\omega;\mathbb{R}^{m\times n}\right) \times W^{1,2}(\omega;\mathbb{R}^{M+1})$ and restrict the space further by imposing the *admissibility condition*

$$\mathbb{Q} := \left\{q \in \mathscr{Q}\ \middle|\ \lambda = \mathscr{L}\bullet\nu \text{ and } \nabla y = \mathbb{I}\bullet\nu\right\}\,, \tag{1.21}$$

where, for almost all $x \in \Omega$, $[\mathscr{L}\bullet\nu](x) := \int_{\mathbb{R}^{m\times n}} \mathscr{L}(F)\nu_x(\mathrm{d}F)$.

Following [FM06], we assume that there are constants $C_0, C_1 > 0$ such that

$$|\partial_t \mathscr{I}(t,q)| \le C_0(C_1 + \mathscr{I}(t,q)) \,. \tag{1.22}$$

We also assume uniform continuity of $t \mapsto \partial_t \mathscr{I}(t,q)$ in the sense that there is $\omega\colon [0,\mathfrak{T}] \to [0,+\infty)$ nondecreasing such that for all $t_1, t_2 \in [0,\mathfrak{T}]$

$$|\partial_t \mathscr{I}(t_1,q) - \partial_t \mathscr{I}(t_2,q)| \le \omega(|t_1 - t_2|) \,. \tag{1.23}$$

Finally, we suppose that $q \mapsto \partial_t \mathscr{I}(t,q)$ is weakly continuous for all $t \in [0,\mathfrak{T}]$.

We seek to analyse the time evolution of a process $q(t) \in \mathbb{Q}$ during the time interval $[0,\mathfrak{T}]$. The following two properties are key ingredients of the so-called energetic solution [MTL02].

(i) *Stability inequality*: for every $t \in [0,\mathfrak{T}]$ and every $\tilde{q} \in \mathbb{Q}$, it holds that

$$\mathscr{I}(t,q(t)) \le \mathscr{I}(t,\tilde{q}) + \mathscr{D}(q(t),\tilde{q}) \,. \tag{1.24}$$

(ii) *Energy balance*: For every $0 \le t \le \mathfrak{T}$,

$$\mathscr{I}(t,q(t)) + \mathrm{diss}(\mathscr{D},q;[0,t]) = \mathscr{I}(0,q(0)) + \int_0^t \partial_t \mathscr{I}(\xi,q(\xi))\,\mathrm{d}\xi \,, \tag{1.25}$$

where

$$\mathrm{diss}(\mathscr{D},q;[s,t]) := \sup\left\{ \sum_{j=1}^{N} \mathscr{D}\left(q\left(t_{j-1}\right), q\left(t_j\right)\right) \;\middle|\; \{t_j\}_{j=0}^{N} \text{ is a partition of } [s,t] \right\}$$

is the *variation* of the dissipation.

Definition 1. The mapping $q\colon [0,\mathfrak{T}] \to \mathbb{Q}$ is an *energetic solution* to the problem $(\mathscr{I},\mathscr{D})$ with the energy functional $\mathscr{I}$ as in (1.19) and the dissipation $\mathscr{D}$ if the stability inequality (1.24) and energy balance (1.25) are satisfied for every $t \in [0,\mathfrak{T}]$.

Further, we define the set of stable states at time $t \in [0,\mathfrak{T}]$ as

$$\mathbb{S}(t) := \{q \in \mathbb{Q};\ \forall \tilde{q} \in \mathbb{Q} : \mathscr{I}(t,q) \le \mathscr{I}(t,\tilde{q}) + \mathscr{D}(q,\tilde{q})\} \,.$$

In particular, we will always assume that the initial condition is stable, i.e., $q_0 \in \mathbb{S}(0)$. The following theorem regarding the existence of an energetic solution can be proved using a general strategy described in [FM06].

Theorem 1. *Let $p > 2$, and let assumptions* (1.4), (1.22), *and* (1.23) *hold. Then there is a process $q\colon [0,\mathfrak{T}] \to \mathbb{Q}$ with $q(t) = (y(t), \nu(t), \lambda(t))$ such that q is an energetic solution according to Definition 1 for a given stable initial condition $q_0 \in \mathbb{Q}$.*

Proof. The proof of this theorem follows a now well-established route and we thus omit any details [MR03]. The argument proceeds via semidiscretisations in time for decreasing time steps, by a limit passage in the stability inequality (1.24) and in the energy equality (1.25); cf. also [FM06] for a general strategy how to prove existence of energetic solutions. $\square$

1.3 Problems involving concentration

The previous result relies on the specific form (1.10) of the thin film energy and on applied Dirichlet boundary conditions. An advantage of this approach is that the analysis remains in the realm of Young measures, and established tools from analysis can be applied to the quasiconvexified problem. This is just possible because minimizing sequences $\{y_k\}$ to $\mathscr{J} J$ are such that $\{W(\nabla y_k\}_{k\in\mathbb{N}}$ is weakly relatively compact in $L^1(\omega)$. Sometimes it is desirable to study problems where concentration effects may appear as well; then Young measures prove to be insufficient and DiPerna-Majda measures are an appropriate tool. This might perhaps happen for energies satisfying (1.26) if we require additionally that $\det\nabla y > 0$ in Ω. We sketch a corresponding framework and give a simple application. It is worth pointing out that while in spirit the approach is the same as the one taken in Subsection 1.2.1, we there start with a specific two-dimensional energy. Here, we consider a class of three-dimensional energy densities satisfying some growth conditions, and then pass to a two-dimensional setting by considering scaled versions.

Our goal is to tailor the relaxation to functions satisfying (1.2) in the situation of a thin film. The key new idea is that we allow W to depend on the inverse of its argument. Specifically, we suppose that W is continuous on regular matrices and that there exist positive constants $c, C > 0$ such that

$$c\left(-1+|F|^p+\left|F^{-1}\right|^p\right) \leq W(F) \leq C\left(1+|F|^p+\left|F^{-1}\right|^p\right) . \tag{1.26}$$

We point out that (1.26) implies (1.2) and that W has polynomial growth in $|F|$ and $\left|F^{-1}\right|$ at infinity. Hence, in our setting we have an L^p bound not only on the deformation gradient but also on its inverse. Different and even negative powers of F (called the Seth-Hill family of strain measures) are frequently used to describe deformation strain, see, e.g., the survey [CR91]. Notice that if $y\colon \Omega \to \mathbb{R}^3$ is a deformation map and its inverse, $y^{-1}\colon y(\Omega) \to \mathbb{R}^3$ is smooth, then $(\nabla y(x))^{-1} = \nabla y^{-1}(y(x))$. Hence, exchanging the role of the reference and the deformed configuration, the growth condition on F^{-1} just expresses that the gradient of the inverse deformation has the same integrability as the gradient of the original deformation.

A simple example of a function satisfying (1.26) is, e.g., a stored energy density describing martensitic materials:

$$W(F) := \min_{i=1,\ldots,M} \left(\left|F^\top F - F_i^\top F_i\right|^2 + \left|F^{-1}F^{-\top} - F_i^{-1}F_i^{-\top}\right|^2\right) ,$$

where $F_i \in \mathbb{R}^{3\times 3}$, $i = 1, \ldots, M$, are positions of the minima of the multiwell energy. Due to the lack of convexity of W, the existence of a minimiser is typically not guaranteed in the Sobolev space $W^{1,p}(\Omega;\mathbb{R}^3)$; we only trace the behaviour of minimising sequences of J. We describe the necessary tools in the next subsection.

1.3.1 DiPerna-Majda measures

Prior to developing the new framework, we sketch the established theory, which is described in greater detail in, for example, [KZ10]. Unless stated otherwise, Ω is an open domain in $\mathbb{R}^n$. The definition of DiPerna-Majda measures involves a compactification; so let us take a separable completely regular algebra $\mathscr{R}$ of continuous bounded functions $\mathbb{R}^{n\times n} \to \mathbb{R}$. We recall that an algebra is *completely regular* if it contains the constants, separates points from closed subsets and is closed with respect to the maximum (Chebyshev) norm. It is known [Eng77, Sect. 3.12.21] that there is a one-to-one correspondence $\mathscr{R} \mapsto \beta_{\mathscr{R}}\mathbb{R}^{n\times n}$ between such subalgebras of bounded continuous functions and metrisable compactifications of $\mathbb{R}^{n\times n}$; by a compactification we mean here a compact set, denoted by $\beta_{\mathscr{R}}\mathbb{R}^{n\times n}$, into which $\mathbb{R}^{n\times n}$ is homeomorphically and densely embedded. For simplicity, we shall not distinguish between $\mathbb{R}^{n\times n}$ and its image in $\beta_{\mathscr{R}}\mathbb{R}^{n\times n}$. Similarly, we do not distinguish between elements of $\mathscr{R}$ and their unique continuous extensions on $\beta_{\mathscr{R}}\mathbb{R}^{n\times n}$. The reader can, for instance, think about a one point compactification corresponding to the algebra of functions which have limits if the norm of its argument diverges to infinity. The other example is a compactification by the sphere generated by functions which have limits along rays arising from the origin.

Let σ be a positive Radon measure on $\bar{\Omega}$, $\sigma \in M(\bar{\Omega})$. We consider a map $\hat{\nu}$ mapping $x \in \bar{\Omega}$ to a Radon measure $\nu_x \in M(\beta_{\mathscr{R}}\mathbb{R}^{n\times n})$. We recall that such a map $\hat{\nu}\colon x \mapsto \hat{\nu}_x$ is weakly* σ-measurable if for any $v_0 \in C_0(\mathbb{R}^{n\times n})$, the mapping $\bar{\Omega} \to \mathbb{R}, x \mapsto \int_{\beta_{\mathscr{R}}\mathbb{R}^{n\times n}} v_0(s)\hat{\nu}_x(\mathrm{d}s)$ is σ-measurable in the usual sense; the space of weakly* measurable functions is denoted $L^\infty_{\mathrm{w}}(\bar{\Omega},\sigma;M(\beta_{\mathscr{R}}\mathbb{R}^{n\times n}))$. If additionally $\hat{\nu}_x$ is a probability measure, $\nu_x \in \mathrm{Prob}(\beta_{\mathscr{R}}\mathbb{R}^{n\times n})$ for σ-a.a. $x \in \bar{\Omega}$, then the collection $\{\hat{\nu}_x\}_{x\in\bar{\Omega}}$ is a Young measure on $(\bar{\Omega},\sigma)$ [You37]; see also [Bal89, Rou97, Val94, Tay97]. Young measures can record oscillations in minimising sequences but not concentration effects; an extension developed by DiPerna and Majda is capable of describing concentration effects as well.

Specifically, DiPerna and Majda [DM87] have shown that for a bounded sequence $\{y_k\}_{k\in\mathbb{N}}$ in $L^p(\Omega;\mathbb{R}^{n\times n})$ with $1 \leq p < +\infty$, there exists a subsequence (not relabelled), a positive Radon measure $\sigma \in M(\bar{\Omega})$ and a Young measure $\hat{\nu}\colon x \to \hat{\nu}_x$ on $(\bar{\Omega},\sigma)$ such that $(\sigma,\hat{\nu})$ is attainable by $\{y_k\}_{k\in\mathbb{N}}$ in the sense that for every $g \in C(\bar{\Omega})$ and for every

$v_0 \in \mathscr{R}$

$$\lim_{k\to\infty}\int_\Omega g(x)v(y_k(x))\mathrm{d}x = \int_{\bar\Omega}\int_{\beta_{\mathscr{R}}\mathbb{R}^{n\times n}} g(x)v_0(s)\hat\nu_x(\mathrm{d}s)\sigma(\mathrm{d}x)\ , \tag{1.27}$$

where

$$v \in \Upsilon^p_{\mathscr{R}}(\mathbb{R}^{m\times n}) := \left\{v_0(1+|\cdot|^p)\ \middle|\ v_0\in\mathscr{R}\right\}\ . \tag{1.28}$$

We remark that it is easy to see that (1.27) can be also written in the form

$$\lim_{k\to\infty}\int_\Omega h(x,y_k(x))\mathrm{d}x = \int_{\bar\Omega}\int_{\beta_{\mathscr{R}}\mathbb{R}^{n\times n}} h_0(x,s)\hat\nu_x(\mathrm{d}s)\sigma(\mathrm{d}x)\ , \tag{1.29}$$

where $h(x,s) := h_0(x,s)(1+|s|^p)$ and $h_0 \in C(\bar\Omega\otimes\beta_{\mathscr{R}}\mathbb{R}^{n\times n})$.

In particular, setting $v_0 = 1 \in \mathscr{R}$ in (1.27), we can see that

$$\lim_{k\to\infty}(1+|y_k|^p)\ =\ \sigma \qquad \text{weakly* in}\ \ M(\bar\Omega)\ . \tag{1.30}$$

We say that $\{y_k\}_{\in\mathbb{N}}$ *generates* $(\sigma,\hat\nu)$ if (1.27) holds. Let us write $\mathscr{DM}^p_{\mathscr{R}}(\Omega;\mathbb{R}^{m\times n})$ for the set of all *DiPerna-Majda measures*, that is, the set of all pairs $(\sigma,\hat\nu)\in M(\bar\Omega)\times L^\infty_{\mathrm{w}}(\bar\Omega,\sigma;M(\beta_{\mathscr{R}}\mathbb{R}^{n\times n}))$ attainable by sequences from $L^p(\Omega;\mathbb{R}^{n\times n})$. Note that, taking $v_0=1$ in (1.27), one can see that these sequences must inevitably be bounded in $L^p(\Omega;\mathbb{R}^{n\times n})$. The explicit description of the elements from $\mathscr{DM}^p_{\mathscr{R}}(\Omega;\mathbb{R}^{m\times n})$ for unconstrained sequences is given in [KR97, Theorem 2] or in [KR99].

Here the energy depends on the deformation gradient and its inverse. We first ignore the latter dependence and return to this central point at the end of this section. We thus consider the subset of $\mathscr{DM}^p_{\mathscr{R}}(\Omega;\mathbb{R}^{m\times n})$ which are generated by $\{\nabla y_k\}_{k\in\mathbb{N}}$ for some bounded $\{y_k\}_{k\in\mathbb{N}}\subset W^{1,p}(\Omega;\mathbb{R}^m)$; this subset is here denoted as $\mathscr{GDM}^p_{\mathscr{R}}(\Omega;\mathbb{R}^{m\times n})$. Elements of $\mathscr{GDM}^p_{\mathscr{R}}(\Omega;\mathbb{R}^{m\times n})$ generated by gradients of mappings with the same trace on $\partial\Omega$ are characterised in the following theorem, which is proved in [KK08]. To formulate the statement, we introduce the notation $d_\sigma\in L^1(\Omega)$ for the absolutely continuous part of σ in the Lebesgue decomposition of σ, with respect to the Lebesgue measure. We recall that Qv denotes the quasiconvex envelope of a function v.

Theorem 2. *Let $\Omega\subset\mathbb{R}^n$ be a bounded Lipschitz domain , $1<p<+\infty$ and $(\sigma,\hat\nu)\in\mathscr{DM}^p_{\mathscr{R}}(\Omega;\mathbb{R}^{m\times n})$. Then then there is a bounded sequence $\{y_k\}_{k\in\mathbb{N}}\subset W^{1,p}(\Omega;\mathbb{R}^m)$ such that $y_k-y_j\in W^{1,p}_0(\Omega;\mathbb{R}^m)$ for any $j,k\in\mathbb{N}$ (i.e. all have the same trace) and $\{\nabla y_k\}_{k\in\mathbb{N}}$ generates $(\sigma,\hat\nu)$ if and only if the following three conditions hold:*

1. There exists $y\in W^{1,p}(\Omega;\mathbb{R}^m)$ such that for Lebesgue-almost every $x\in\Omega$

$$\nabla y(x) = d_\sigma(x)\int_{\beta_{\mathscr{R}}\mathbb{R}^{n\times n}}\frac{s}{1+|s|^p}\hat\nu_x(\mathrm{d}s)\ . \tag{1.31}$$

2. For all $v\in\Upsilon^p_{\mathscr{R}}(\mathbb{R}^{m\times n})$ as defined in (1.28)*, it holds that Lebesgue-almost everywhere*

$$Qv(\nabla y(x)) \le d_\sigma(x)\int_{\beta_{\mathscr{R}}\mathbb{R}^{n\times n}}\frac{v(s)}{1+|s|^p}\hat\nu_x(\mathrm{d}s)\ . \tag{1.32}$$

3. For σ-almost all $x\in\bar\Omega$ and all $v\in\Upsilon^p_{\mathscr{R}}(\mathbb{R}^{m\times n})$ with $Qv>-\infty$ it holds that

$$0\le\int_{\beta_{\mathscr{R}}\mathbb{R}^{n\times n}\setminus\mathbb{R}^{n\times n}}\frac{v(s)}{1+|s|^p}\hat\nu_x(\mathrm{d}s)\ . \tag{1.33}$$

1.3.2 DiPerna-Majda measures depending on the inverse

We now consider the case where the energy depends on the deformation gradient and its inverse. An existence result for the DiPerna-Majda measures generated by functions with this dependence is required; we state the equivalent to (1.27) for this case. In what follows, $\mathbb{R}^{n\times n}_{\rm inv}$ denotes the set of invertible matrices. The proof of the following theorem is exactly the same as the proof of [Rou97, Theorem 3.2.12].

Theorem 3. *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, for some p with $1\le p<+\infty$. Then there are a subsequence of $\{Y_k\}_{k\in\mathbb{N}}$ (not relabeled), $\pi\in M(\bar\Omega)$ and $\hat\mu\in L^\infty_{\rm w}(\bar\Omega,\pi;M(\beta_{\mathscr{R}}\mathbb{R}^{n\times n}))$ such that for every $g\in C(\bar\Omega)$ and every $v(s)=v_1(s)(1+|s|^p+\left|s^{-1}\right|^p)$ with $v_1\colon\mathbb{R}^{n\times n}_{\rm inv}\to\mathbb{R}$ which can be continuously extended to $v_0\in\mathscr{R}$, it holds that*

$$\lim_{k\to\infty}\int_\Omega g(x)v(Y_k(x))\,\mathrm{d}x=\int_{\bar\Omega}\int_{\beta_{\mathscr{R}}\mathbb{R}^{n\times n}}g(x)v_0(s)\hat\mu_x(\mathrm{d}s)\,\pi(\mathrm{d}x)\;. \tag{1.34}$$

Moreover, $\pi=w^*-\lim_{k\to\infty}1+|Y_k|^p+\left|Y_k^{-1}\right|^p$ in $M(\bar\Omega)$.

We will denote the set of pairs $(\pi,\hat\mu)$ defined in Theorem 3 by $\mathscr{DM}^{p,-p}_{\mathscr{R}}(\Omega;\mathbb{R}^{n\times n})$ and its subset generated by gradients of functions from $W^{1,p}(\Omega;\mathbb{R}^n)$, i.e., if $Y_k:=\nabla y_k$, by $\mathscr{GDM}^{p,-p}_{\mathscr{R}}(\Omega;\mathbb{R}^{n\times n})$.

The classic DiPerna-Majda measures are fully characterised, as stated in Theorem 2. For measures depending on the inverse as defined in Theorem 3, there is no full characterisation available; this is since the nonlinearity introduced by the inverse rules out the application of existing tools for the characterisation of DiPerna-Majda measures. We now give a partial characterisation. Taking $v(s):=1+|s|^p$, we have $v_0(s)=1$ in (1.27); we claim that

$$v_0(s):=\begin{cases}\frac{1+|s|^p}{1+|s|^p+\left|s^{-1}\right|^p} & \text{if } s\in\mathbb{R}^{n\times n}_{\rm inv}\\ 0 & \text{otherwise}\end{cases} \tag{1.35}$$

in (1.34). To see this, we set

$$v_1(s)=\frac{1+|s|^p}{1+|s|^p+|s^{-1}|^p}$$

and notice that

$$\lim_{\substack{|s^{-1}|\to\infty\\ |s|\text{ bounded}}}v_1(s)=0$$

exists; thus we can first extend v_1 by continuity to the set of non-invertible matrices and obtain v_0 as in (1.35). Comparing (1.27) and (1.34), we then find for π-almost all $x\in\bar\Omega$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\pi}(x)=\int_{\beta_{\mathscr{R}}\mathbb{R}^{n\times n}}\frac{1+|s|^p}{1+|s|^p+|s^{-1}|^p}\hat\mu_x(\mathrm{d}s)\;. \tag{1.36}$$

Using this and choosing arbitrary $v_0\in\mathscr{R}$ we obtain

$$\int_{\beta_{\mathscr{R}}\mathbb{R}^{n\times n}}v_0(s)\hat\nu_x(\mathrm{d}s)=\left(\int_{\beta_{\mathscr{R}}\mathbb{R}^{n\times n}}\frac{1+|s|^p}{1+|s|^p+|s^{-1}|^p}\hat\mu_x(\mathrm{d}s)\right)^{-1}\int_{\beta_{\mathscr{R}}\mathbb{R}^{n\times n}}\frac{v_0(s)(1+|s|^p)}{1+|s|^p+|s^{-1}|^p}\hat\mu_x(\mathrm{d}s)\;. \tag{1.37}$$

To ensure that the DiPerna-Majda measure is generated by a sequence of gradients (and their inverses), we use this characterisation in terms of $(\sigma,\hat\nu)$. Namely, we require that the DiPerna-Majda measure $(\sigma,\hat\nu)$ defined by (1.36), (1.37) must belong to $\mathscr{GDM}^p_{\mathscr{R}}(\Omega;\mathbb{R}^{m\times n})$; that is, the conditions in Theorem 2 must be fulfilled. We remark that then the gradient of the macroscopic deformation ∇y can be expressed for almost all $x\in\Omega$ as

$$\nabla y(x)=d_\pi(x)\int_{\beta_{\mathscr{T}}\mathbb{R}^{n\times n}_{\rm inv}}\frac{s}{1+|s|^p+|s^{-1}|^p}\hat\mu_x(\mathrm{d}s)\;, \tag{1.38}$$

where d_π is the density of the absolutely continuous part of π with respect to the Lebesgue measure.

Then the relaxation of J reads

$$\text{minimise}\int_{\bar\Omega}\int_{\beta_{\mathscr{R}}\mathbb{R}^{n\times n}_{\rm inv}}\frac{W(s)}{1+|s|^p+|s^{-1}|^p}\hat\mu_x(\mathrm{d}s)\,\pi(\mathrm{d}x)\;, \tag{1.39}$$

where $(\pi, \hat{\mu}) \in \mathscr{GDM}^{p,-p}_{\mathscr{R}}(\Omega; \mathbb{R}^{n\times n})$, where $\hat{\mu}_x$ is supported on the set of matrices with positive determinant for π-almost all $x \in \bar{\Omega}$.

1.3.3 Application to a thin film model

We now describe a setting for the analysis of thin martensitic films. A similar framework has been analysed by Bocea [Boc08]; while the description of the thin film bears many resemblances, there are two crucial differences. We allow the energy to depend on the inverse, with the growth condition as in (1.26). This has the benefit that the important physical constraint (1.2) is satisfied. However, a price to pay is we cannot apply a decomposition lemma as used by Bocea [Boc08]; it is an open problem whether a decomposition lemma holds for measures generated by gradients and their inverses. We recall the standard decomposition lemma which can be found in [FMP98].

Lemma 1. *Let $1 < p < +\infty$ and $\Omega \subset \mathbb{R}^n$ be an open bounded set and let $\{u_k\}_{k\in\mathbb{N}} \subset W^{1,p}(\Omega; \mathbb{R}^m)$ be bounded. Then there is a subsequence $\{u_j\}_{j\in\mathbb{N}}$ and a sequence $\{z_j\}_{j\in\mathbb{N}} \subset W^{1,p}(\Omega; \mathbb{R}^m)$ such that*

$$\lim_{j\to\infty} \left|\{x \in \Omega;\ z_j(x) \neq u_j(x) \text{ or } \nabla z_j(x) \neq \nabla u_j(x)\}\right| = 0 \tag{1.40}$$

and $\{|\nabla z_j|^p\}_{j\in\mathbb{N}}$ is relatively weakly compact in $L^1(\Omega)$. In particular, $\{\nabla u_j\}$ and $\{\nabla z_j\}$ generate the same Young measure.

It is, however, not known if an analogous lemma hold if we require also a bound on the gradient inverse. Thus we cannot rule out concentration effects and have to resort to a variant of DiPerna-Majda measures as described in Subsection 1.3.2. (The special case discussed in Subsection 1.2.1, with the specific energy given in (1.10), is an example where we have shown that no concentrations occur, so there the framework of Young measures is suitable).

We recall that $\omega \subset \mathbb{R}^2$ is an open, bounded domain with Lipschitz boundary, and that we set $I := (0,1)$ and $\Omega_\varepsilon := \omega \times \varepsilon I$ as the reference state for the space occupied by a specimen. Further, $y_\varepsilon\colon \Omega_\varepsilon \to \mathbb{R}^3$ is the deformation and $u_\varepsilon\colon \Omega_\varepsilon \to \mathbb{R}^3$ is the displacement, which are related to each other via the identity $y_\varepsilon(x^\varepsilon) = x^\varepsilon + u_\varepsilon(x^\varepsilon)$, where $x^\varepsilon \in \Omega_\varepsilon$. Hence the deformation gradient is $F_\varepsilon := \nabla y_\varepsilon = \mathbb{I} + \nabla u_\varepsilon$. Here, $\mathbb{I} \in \mathbb{R}^{3\times 3}$ is the identity matrix.

The total stored energy in the bulk occupying, in its reference configuration, the domain Ω_ε, is then

$$V(y_\varepsilon) := \int_{\Omega_\varepsilon} W(\nabla y_\varepsilon(x^\varepsilon))\,\mathrm{d}x^\varepsilon\ . \tag{1.41}$$

Here the bulk free energy density W is a function $W\colon \mathbb{R}^{n\times n}_{\mathrm{inv}+} \to \mathbb{R}$, taking the deformation gradient as its argument. In reality, W also depends on the temperature, but we restrict here the analysis to the isothermal case of a temperature below the critical temperature, since the difficulty of non-convexity appears here as isolated as possible from other effects. Then several martensitic variants coexist, and this is what we want to capture.

The usual symmetry requirements will be made, namely frame indifference

$$W(QF) = W(F) \text{ for every } Q \in \mathrm{SO}(3) \text{ and } F \in \mathbb{R}^{n\times n}_{\mathrm{inv}+} \tag{1.42}$$

and crystalline symmetry

$$W(FP) = W(F) \text{ for every } P \in \mathscr{P} \text{ and } F \in \mathbb{R}^{n\times n}_{\mathrm{inv}+}\ , \tag{1.43}$$

here $\mathscr{P}$ denotes the point group of the austenitic phase. The set of minimisers of W is given by the martensitic variants $U_1, \ldots, U_M$. The frame indifference (1.42) then implies that W is minimised on $\cup_{j=1}^M \mathrm{SO}(3)U_j$, the union of the orbits of U_j under the operation of $\mathrm{SO}(3)$ from the left.

It is convenient to consider $\Omega := \omega \times I$ which originates from Ω_ε via dilatation by $\frac{1}{\varepsilon}$ in the direction of the third component. So, if the coordinates in Ω_ε are $(x_1^\varepsilon, x_2^\varepsilon, x_3^\varepsilon)$, then the coordinates in Ω are (x_1, x_2, x_3) with

$$x_1 = x_1^\varepsilon, \qquad x_2 = x_2^\varepsilon, \qquad x_3 = \frac{1}{\varepsilon} x_3^\varepsilon \; .$$

The deformation $y_\varepsilon\colon \Omega_\varepsilon \to \mathbb{R}^3$ then gives in a natural way rise to the rescaled deformation $y\colon \Omega \to \mathbb{R}^3$ via $y(x) = y_\varepsilon(x^\varepsilon(x))$. A rescaling of the energy (1.41) by a factor $\frac{1}{\varepsilon}$ yields then

$$V_\varepsilon(y) := \int_\Omega W\left(\nabla_{1,2} y(x) \;\middle|\; \tfrac{1}{\varepsilon}\nabla_3 y(x)\right) \mathrm{d}x \; ; \tag{1.44}$$

we recall that $\nabla_{1,2}$ is the 3×2 matrix of partial derivatives $y_{j,k} = \frac{\partial y_j}{\partial x_k}$ with $j \in \{1,2,3\}$ and $k \in \{1,2\}$ and $\nabla_3 y = y_{,3}$ is the (column) vector containing the derivatives of y with respect to x_3 and $(F|f)$ denotes the 3×3 matrix formed of the 3×2 matrix F as the first two columns and the vector f as the third column.

We assume that W satisfies (1.26), that is,

$$c(-1 + |F|^p + \left|F^{-1}\right|^p) \le W(F) \le C(1 + |F|^p + \left|F^{-1}\right|^p)$$

for some $p \in \mathbb{N}$. This is a central difference to the work in [Boc08], where the growth condition is in terms of F alone rather than both F and F^{-1}.

Definition 2 (Scaled DiPerna-Majda measures). Let $A = (a_1|a_2|a_3) \in \mathbb{R}^{3\times 3}$ be given. Let $\{y_k\}_{k\in\mathbb{N}}$ be a sequence of functions with affine boundary data in the sense that $y_k(x) = A^{\varepsilon_k} x := (a_1|a_2|\varepsilon_k a_3)x$ for $x \in \partial\omega \times I$. Suppose further that $\left(\nabla_{1,2} y_k(x) \;\middle|\; \frac{1}{\varepsilon}\nabla_3 y_k(x)\right)$ and $\left(\nabla_{1,2} y_k(x) \;\middle|\; \frac{1}{\varepsilon}\nabla_3 y_k(x)\right)^{-1}$ are both uniformly bounded in $L^p(\Omega;\mathbb{R}^{n\times n})$, for some p with $1 \le p < +\infty$. Then there is a subsequence which generates a measure $(\pi,\hat\mu) \in \mathscr{DM}^{p,-p}_{\mathscr{R}}(\Omega;\mathbb{R}^{n\times n})$; this measure is called a *scaled DiPerna-Majda measure*.

The existence of a scaled DiPerna-Majda measure follows directly from Theorem 3 .

As an application of the theory developed, we formulate the following result. A related result was given in [Boc08].

Proposition 3. *Let W satisfy the growth condition* (1.26)*. Let $\{\varepsilon_k\}_{k\in\mathbb{N}}$ be a sequence of real numbers with $\varepsilon_k \to 0$ as $k \to \infty$ and $\{y_k\}_{k\in\mathbb{N}}$ be a sequence of functions with affine boundary data, $y_k(x) = A^{\varepsilon_k} x := (a_1|a_2|\varepsilon_k a_3)x$ for $x \in \partial\omega \times I$. Suppose that $\{y_k\}_{k\in\mathbb{N}}$ is a minimising sequence for* (1.44)*, in the sense that*

$$V_\varepsilon(y_k) = \int_\Omega W\left(\nabla_{1,2} y_k(x) \;\middle|\; \tfrac{1}{\varepsilon_k}\nabla_3 y_k(x)\right) \mathrm{d}x < I_k + \varepsilon_k \; ,$$

where

$$I_k := \inf\left\{ V_{\varepsilon_k}(y) \;\middle|\; y \in W^{1,p}(\Omega,\mathbb{R}^3), y(x) = A^{\varepsilon_k} x \text{ for } x \in \partial\omega \times I \right\} \; .$$

Then a subsequence of $\{y_k\}_{k\in\mathbb{N}}$ (not relabeled) generates a scaled DiPerna-Majda measure $(\pi,\hat\mu) \in \mathscr{DM}^{p,-p}_{\mathscr{R}}(\Omega;\mathbb{R}^{n\times n})$, and $(\pi,\hat\mu)$ minimises the effective film energy

$$\int_{\bar\Omega} \int_{\beta_{\mathscr{R}} \mathbb{R}^{n\times n}_{\mathrm{inv}}} \frac{W(s)}{1 + |s|^p + |s^{-1}|^p} \, \hat\mu_x(\mathrm{d}s) \, \pi(\mathrm{d}x) \; , \tag{1.45}$$

among all scaled gradient measures in $\mathscr{DM}^{p,-p}_{\mathscr{R}}(\Omega;\mathbb{R}^{n\times n})$.

Proof. The growth assumption (1.26) yields that $\left(\nabla_{1,2} y_k(x) \;\middle|\; \frac{1}{\varepsilon}\nabla_3 y_k(x)\right)$ and $\left(\nabla_{1,2} y_k(x) \;\middle|\; \frac{1}{\varepsilon}\nabla_3 y_k(x)\right)^{-1}$ are both uniformly bounded in $L^p(\Omega;\mathbb{R}^{n\times n})$. The existence of a scaled DiPerna-Majda measure follows then from Theorem 3, and it is a standard fact that minimising sequences $\{y_k\}_{k\in\mathbb{N}}$ generate a minimiser of the relaxed functional, which is here (1.45).

1.4 Open problems

The analysis of problems satisfying the physically natural growth assumption (1.2) is currently not well developed; we highlight some avenues of possible future research.

For the full vectorial case (i.e. $m, n > 1$), in [BKP11], a relaxation theory in terms of Young measures is given. One challenge is the characterisation of the measures involved; a second one is the inclusion of possible concentrations. This would lead to a description of DiPerna-Majda measures depending on the inverse, as introduced in Section 1.3. There again, the characterisation of the measures obtained is a mathematical problem in its own right. A further problem is that at present, we do not know under which conditions a decomposition lemma holds (see Subsection 1.3.3).

From the point of view of applications, the existence theory for models with energies satisfying the growth assumption (1.2) is a natural source of problems. In addition, the analysis of limits is open; for example, which thin-film energies of type (1.2) can be obtained from three-dimensional equations, in the limit of vanishing film thickness? Similarly as in bulk materials positivity of the determinant plays a crucial role, not only the length of the normal but also its orientation is important in thin films. We refer to [CGM11] for a recent result in this direction using the notion of surface polyconvexity.

References

[ABP91] Emilio Acerbi, Giuseppe Buttazzo, and Danilo Percivale. A variational definition of the strain energy for an elastic string. *J. Elasticity*, 25(2):137–148, 1991.

[AHM08] Omar Anza Hafsa and Jean-Philippe Mandallena. Relaxation theorems in nonlinear elasticity. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 25(1):135–148, 2008.

[Bal89] J. M. Ball. A version of the fundamental theorem for Young measures. In M. Rascle, D. Serre, and M. Slemrod, editors, *PDEs and continuum models of phase transitions (Nice, 1988)*, pages 207–215. Springer, Berlin, 1989.

[Bal77] John M. Ball. Convexity conditions and existence theorems in nonlinear elasticity. *Arch. Rational Mech. Anal.*, 63(4):337–403, 1976/77.

[BB00] Hafedh Ben Belgacem. Relaxation of singular functionals defined on Sobolev spaces. *ESAIM Control Optim. Calc. Var.*, 5:71–85 (electronic), 2000.

[BJ87] J. M. Ball and R. D. James. Fine phase mixtures as minimizers of energy. *Arch. Rational Mech. Anal.*, 100(1):13–52, 1987.

[BJ99] K. Bhattacharya and R. D. James. A theory of thin films of martensitic materials with applications to microactuators. *J. Mech. Phys. Solids*, 47(3):531–576, 1999.

[BK11] S. Bartels and M. Kružík. An efficient approach to the numerical solution of rate-independent problems with nonconvex energies. *Multiscale Model. Simul.*, 9(3):1276–1300, 2011.

[BKP11] Barbora Benešová, Martin Kružík, and Gabriel Pathó. Young measures supported on invertible matrices. http://arxiv.org/abs/1103.2859, 2011.

[Boc08] Marian Bocea. A justification of the theory of martensitic thin films in the absence of an interfacial energy. *J. Math. Anal. Appl.*, 342(1):485–496, 2008.

[CGM11] Philippe G. Ciarlet, Radu Gogu, and Cristinel Mardare. A notion of polyconvex function on a surface suggested by nonlinear shell theory. *C. R., Math., Acad. Sci. Paris*, 349(21-22):1207–1211, 2011.

[Cia88] Philippe G. Ciarlet. *Mathematical elasticity. Vol. I*, volume 20 of *Studies in Mathematics and its Applications*. North-Holland Publishing Co., Amsterdam, 1988. Three-dimensional elasticity.

[CR91] A. Curnier and L. Rakotomanana. Generalized strain and stress measures: critical survey and new results. *Engrg. Trans.*, 39(3-4):461–538 (1992), 1991.

[Dac89] Bernard Dacorogna. *Direct methods in the calculus of variations*, volume 78 of *Applied Mathematical Sciences*. Springer-Verlag, Berlin, 1989.

[DM87] Ronald J. DiPerna and Andrew J. Majda. Oscillations and concentrations in weak solutions of the incompressible fluid equations. *Comm. Math. Phys.*, 108(4):667–689, 1987.

[Eng77] Ryszard Engelking. *General topology*. PWN—Polish Scientific Publishers, Warsaw, 1977. Translated from the Polish by the author, Monografie Matematyczne, Tom 60. [Mathematical Monographs, Vol. 60].

[FL07] Irene Fonseca and Giovanni Leoni. *Modern methods in the calculus of variations: L^p spaces*. Springer Monographs in Mathematics. Springer, New York, 2007.

[FM06] Gilles Francfort and Alexander Mielke. Existence results for a class of rate-independent material models with nonconvex elastic energies. *J. Reine Angew. Math.*, 595:55–91, 2006.

[FMP98] Irene Fonseca, Stefan Müller, and Pablo Pedregal. Analysis of concentration and oscillation effects generated by gradients. *SIAM J. Math. Anal.*, 29(3):736–756, 1998.

[FP04] Lorenzo Freddi and Roberto Paroni. A 3D–1D Young measure theory of an elastic string. *Asymptot. Anal.*, 39(1):61–89, 2004.

[KK08] Agnieszka Kałamajska and Martin Kružík. Oscillations and concentrations in sequences of gradients. *ESAIM Control Optim. Calc. Var.*, 14(1):71–104, 2008.

[KMR05] Martin Kružík, Alexander Mielke, and Tomáš Roubíček. Modelling of microstructure and its evolution in shape-memory-alloy single-crystals, in particular in CuAlNi. *Meccanica*, 40(4-6):389–418, 2005.

[KP94] David Kinderlehrer and Pablo Pedregal. Gradient Young measures generated by sequences in Sobolev spaces. *J. Geom. Anal.*, 4(1):59–90, 1994.

[KR97] Martin Kružík and Tomáš Roubíček. On the measures of DiPerna and Majda. *Math. Bohem.*, 122(4):383–399, 1997.

[KR99] Martin Kružík and Tomáš Roubíček. Optimization problems with concentration and oscillation effects: Relaxation theory and numerical approximation. *Numer. Funct. Anal. Optimization*, 20(5-6):511–530, 1999.

[Kru98] Martin Kružík. Numerical approach to double well problems. *SIAM J. Numer. Anal.*, 35(5):1833–1849, 1998.

[KZ10] Martin Kružík and Johannes Zimmer. Evolutionary problems in nonreflexive spaces. *ESAIM Control Optim. Calc. Var.*, 16(1):1–22, 2010.

[KZ11] Martin Kružík and Johannes Zimmer. A model of shape memory alloys taking into account plasticity. *IMA J. Appl. Math.*, 76(1):193–216, 2011.

[Mor08] Charles B. Morrey, Jr. *Multiple integrals in the calculus of variations*. Classics in Mathematics. Springer-Verlag, Berlin, 2008. Reprint of the 1966 edition [MR0202511].

[MR03] Alexander Mielke and Tomáš Roubíček. A rate-independent model for inelastic behavior of shape-memory alloys. *Multiscale Model. Simul.*, 1(4):571–597 (electronic), 2003.

[MTL02] Alexander Mielke, Florian Theil, and Valery I. Levitas. A variational formulation of rate-independent phase transformations using an extremum principle. *Arch. Ration. Mech. Anal.*, 162(2):137–177, 2002.

[Mül99] Stefan Müller. Variational models for microstructure and phase transitions. In *Calculus of variations and geometric evolution problems (Cetraro, 1996)*, volume 1713 of *Lecture Notes in Math.*, pages 85–210. Springer, Berlin, 1999.

[Rou97] Tomáš Roubíček. *Relaxation in optimization theory and variational calculus*, volume 4 of *de Gruyter Series in Nonlinear Analysis and Applications*. Walter de Gruyter & Co., Berlin, 1997.

[Tay97] Michael E. Taylor. *Partial differential equations. III*, volume 117 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 1997. Nonlinear equations, Corrected reprint of the 1996 original.

[Val94] M. Valadier. A course on Young measures. In *Workshop on Measure Theory and Real Analysis (Grado, 1993), Rend. Istit. Mat. Univ. Trieste*, volume 26, pages 349–394, 1994.

[You37] L. C. Young. Generalized curves and the existence of an attained absolute minimum in the calculus of variations. *Comptes Rendus de la Société des Sciences et des Lettres de Varsovie, Classe III*, (30):212–234, 1937.

Acknowledgment: The work of MK was partially supported by the grant P201/10/0357 (GA ČR), the work of JZ was partially supported by EPSRC (EP/H05023X/1). Both authors gratefully acknowledge funding by the Royal Society (JP080789).