Shape memory alloys as gradient-polyconvex materials

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Abstract

We show existence of an energetic solution to a model of shape memory alloys in which the elastic energy is described by means of a gradient-polyconvex functional. This allows us to show existence of a solution based on weak continuity of nonlinear minors of deformation gradients in Sobolev spaces. Resulting deformations are orientation-preserving and injective everywhere in a domain representing the specimen.

Key Words: Gradient polyconvexity, invertibility of deformations, orientation-preserving mappings, shape memory alloys

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1 Introduction

Hyperelasticity is a special area of Cauchy elasticity where one assumes that the first Piola-Kirchhoff stress tensor $S$ possesses a potential (called stored energy density) $W : \mathbb{R}^{3 \times 3} \to [-w, \infty]$, for some $w \geq 0$. In other words,

$$S := \frac{\partial W(F)}{\partial F}$$

(1.1)
on its domain, where $F \in \mathbb{R}^{3 \times 3}$ is such that $\det F > 0$. This concept emphasizes that all work done by external loads on the specimen is stored in it. The principle of frame-indifference requires that $W$ satisfies for all $F \in \mathbb{R}^{3 \times 3}$ and all proper rotations $R \in \text{SO}(3)$

$$W(F) = W(RF) = \tilde{W}(F^\top F) = \tilde{W}(C),$$

where $C := F^\top F$ is the right Cauchy-Green strain tensor and $\tilde{W} : \mathbb{R}^{3 \times 3} \to [-w, \infty]$. Additionally, every elastic material is assumed to resist extreme compression, which is modeled by assuming

$$W(F) \to +\infty \text{ if } \det F \to 0_+.$$  (1.2)
Let the reference configuration be a bounded Lipshitz domain \( \Omega \subset \mathbb{R}^3 \). If we consider a deformation \( y : \bar{\Omega} \to \mathbb{R}^3 \), which is a mapping that assigns to each point in the closure of the reference configuration \( \bar{\Omega} \) its position after deformation, solutions to corresponding elasticity equations can be formally found by minimizing an energy functional

\[
I(y) := \int_{\Omega} W(\nabla y(x)) \, dx - \ell(y)
\]  

over a class of admissible deformations. Here \( \ell \) is a functional on the set of deformations expressing (in a simplified way) the work of external loads on the specimen and \( \nabla y \) is the deformation gradient which quantifies the strain. We only allow for deformations which are orientation-preserving, i.e. if \( a, b, c \in \mathbb{R}^3 \) satisfy \( (a \times b) \cdot c > 0 \), then \( (Fa \times Fb) \cdotFc > 0 \) for every \( F := \nabla y(x) \) and \( x \in \Omega \). Which means that \( \det F > 0 \). This condition can be expressed by extending \( W \) by infinity to matrices with nonpositive determinants,

\[
W(F) := +\infty \text{ if } \det F \leq 0.
\]  

In view of (1.1), (1.2), and (1.4) we see that \( W : \mathbb{R}^{3\times3} \to [-w, +\infty] \), for some \( w \geq 0 \), is continuous in the sense that if \( F_k \to F \) in \( \mathbb{R}^{3\times3} \) for \( k \to +\infty \), then \( \lim_{k \to +\infty} W(F_k) = W(F) \). Furthermore, \( W \) is differentiable on the set of matrices with positive determinants.

A key question immediately appears: Under which conditions does the functional \( I \) in (1.3) possess minimizers? Relying on the direct method of the calculus of variations, the usual approach to address this question is to study (weak) lower semicontinuity of the functional \( I \) on appropriate Banach spaces containing the admissible deformations. For definiteness, we assume that \( y \mapsto -\ell(y) \) is weakly sequentially lower semicontinuous. Thus the question reduces do a discussion of the assumptions on \( W \). It is well known that (1.2) prevents us from assuming convexity of \( W \). See e.g. [12] or the recent review [6] for a detailed exposition of weak lower semicontinuity. In his seminal contribution [1], J.M. Ball defined a polyconvex stored energy density \( W \) by assuming that there is a convex and lower semicontinuous function \( \bar{W} : \mathbb{R}^1 \to [-w, +\infty] \) such that

\[
W(F) := \bar{W}(F, \text{Cof } F, \det F).
\]

Here \( \text{Cof } F \) is the cofactor matrix of \( F \), which for \( F \) being invertible satisfies Cramer’s rule

\[
\text{Cof } F = (\det F)F^{-\top}.
\]

It is well-known that polyconvexity is satisfied for a large class of constitutive functions and allows for existence of minimizers of \( I \) under (1.2) and (1.4). On the other hand, there are still situations where polyconvexity cannot be adopted. A prominent example are shape-memory alloys, see e.g. [1, 8, 21], where \( W \) has the so-called multi-well structure. Namely, there is a high-temperature phase called austenite, which is usually of cubic symmetry, and a low-temperature phase called martensite, which is less symmetric and exists in more variants, e.g., in three for the tetragonal structure (NiMnGa) or in twelve for the monoclinic one (NiTi). We can assume that

\[
W(F) := \min_{0 \leq i \leq M} W_i(F),
\]

where \( W_i : \mathbb{R}^{3\times3} \to [-w_i, +\infty], w_i \geq 0 \), is the stored energy density of the \( i \)-th variant of martensite if \( i > 0 \), and \( W_0 \) is the stored energy density of the austenite. For every admissible \( i \), \( W_i(F) = -w_i \) if and only if \( F = RF_i \) for a given matrix \( F_i \in \mathbb{R}^{3\times3} \) and an arbitrary proper rotation \( R \in \text{SO}(3) \).
Let us emphasize that (1.5) ruins even generalized notions of convexity as e.g. rank-one convexity (we recall that rank-one convex functions are convex on line segments whose endpoints differ by a rank-one matrix and that rank-one convexity is a necessary condition for polyconvexity; cf. [12], for instance). Namely, it is observed (see e.g. [4, 8]) that $w_i = w_j$ whenever $i, j \neq 0$ and that there is a proper rotation $R_{ij}$ such that $\operatorname{rank}(R_{ij}F_i - F_j) = 1$. Hence, generically, $W(R_{ij}F_i) = W(F_j) = -w_i$, but $W(F) > -w_i$ if $F$ is on the line segment between $R_{ij}F_i$ and $F_j$; however, not having a convexity property at hand that implied existence of minimizers is in accordance with experimental observations for these alloys.

Indeed, nonexistence of a minimizer corresponds to the formation of microstructure of strain-states which is mathematically manifested via faster and faster oscillation of deformation gradients in minimizing sequences driving the functional $I$ to its infimum. One can then formulate a minimization problem for a lower semicontinuous envelope of $I$, the so-called relaxation, see, e.g., [12]. Such a relaxation yields information of the effective behaviour of the material and on the set of possible microstructures. Thus relaxation is not only an important tool for mathematical analysis, but also for applications. For numerical considerations it is a challenging problem, because the relaxation formula is generically not obtained in a closed form. Further difficulties come from the fact that a sound mathematical relaxation theory is developed only if $W$ has $p$-growth; that is, for some $c > 1$, $p \in (1, + \infty)$ and all $F \in \mathbb{R}^{3 \times 3}$ the inequality

$$
\frac{1}{c}(|F|^p - 1) \leq W(F) \leq c(1 + |F|^p)
$$

is satisfied, which in particular implies that $W < + \infty$. We refer, however, to [6, 11, 18] for results allowing for infinite energies. Nevertheless, these works include other assumptions which severely restrict their usage. Let us point out that the right Cauchy-Green strain tensor $F^\top F$ maps $\text{SO}(3)F$ as well as $(\text{O}(3) \setminus \text{SO}(3))F$ to the same point. Here $O(3)$ are orthogonal matrices with determinant $\pm 1$. Thus, for example, $F \mapsto |F^\top F - I|$ is minimized on two energy wells, on $\text{SO}(3)$ and also on $O(3) \setminus \text{SO}(3)$. However, the latter set is not acceptable in elasticity because the corresponding minimizing affine deformation is a mirror reflection. In order to distinguish between these two wells, it is necessary to incorporate $\det F$ in the model properly.

Besides relaxation, another approach guaranteeing existence of minimizers is to resort to non-simple materials, i.e., materials whose stored energy density depends (in a convex way) on higher deformation gradients. This idea goes back to Toupin [23, 24] and is used in many works from then on [3, 13, 15, 22], including work on shape-memory alloys [2, 5]. Simple examples are functionals of the form

$$
I(y) := \int_\Omega W(\nabla y(x)) + \varepsilon|\nabla^2 y(x)|^p \, dx - \ell(y),
$$

where $\varepsilon > 0$. Obviously, the second-gradient term brings additional compactness to the problem, which allows to require only strong lower semicontinuity of the term

$$
\nabla y \mapsto \int_\Omega W(\nabla y(x)) \, dx
$$

for existence of minimizers.

Here we follow a different approach recently suggested in [7], which is a natural extension of polyconvexity exploiting weak continuity of minors in Sobolev spaces. Instead of the full second gradient, it is assumed that the stored energy of the material depends on the deformation gradient
\( \nabla y \) and on gradients of nonlinear minors of \( \nabla y \), i.e., on \( \nabla \text{Cof} \nabla y \) and on \( \nabla [\det \nabla y] \). The corresponding functionals are then called gradient polyconvex. While we assume convexity of the stored energy density in the two latter terms, this is not assumed in the \( \nabla y \) variable. The advantage is that minimizers are elements of Sobolev spaces \( W^{1,p}(\Omega; \mathbb{R}^3) \) and no higher regularity is required.

The following example is inspired from [7]. It shows that there are maps with smooth nonlinear minors whose deformation gradient is \textit{not} a Sobolev map. Hence, gradient polyconvex energies are more general than second-gradient ones.

**Example 1.1.** Let \( \Omega = (0, 1)^3 \). For functions \( f, g : (0, 1) \to (0, +\infty) \) to be specified later, let us consider the deformation

\[
y(x_1, x_2, x_3) := (x_1, x_2 f(x_1), x_3 g(x_1)).
\]

Then

\[
\nabla y(x_1, x_2, x_3) = \begin{pmatrix}
1 & 0 & 0 \\
x_2 f'(x_1) & f(x_1) & 0 \\
x_3 g'(x_1) & 0 & g(x_1)
\end{pmatrix},
\]

\[
\text{Cof} \nabla y(x_1, x_2, x_3) = \begin{pmatrix}
f(x_1) g(x_1) & -x_2 f'(x_1)g(x_1) & -x_3 f(x_1)g'(x_1) \\
0 & g(x_1) & 0 \\
0 & 0 & f(x_1)
\end{pmatrix}
\]

and

\[
\det \nabla y(x_1, x_2, x_3) = f(x_1)g(x_1) > 0.
\]

Finally, the non-zero entries of \( \nabla^2 y(x_1, x_2, x_3) \) are

\[
x_2 f''(x_1), \quad f'(x_1), \quad x_3 g''(x_1), \quad g'(x_1).
\]

Note that we have in particular

\[
|\nabla^2 y(x_1, x_2, x_3)| \geq |x_2||f''(x_1)|.
\]

Any functions \( f, g \) such that \( y \in W^{1,p}(\Omega; \mathbb{R}^3) \), \( \text{Cof} \nabla y \in W^{1,3}(\Omega; \mathbb{R}^{3\times 3}) \), \( \det \nabla y \in W^{1,r}(\Omega; (0, \infty)) \), \( (\det \nabla y)^{-s} \in L^1(\Omega) \) for some \( p, q, r \geq 1 \) and \( s > 0 \), but such that one of the quantities in (1.6) is \textit{not} a function in \( L^p(\Omega) \) yield a useful example since then \( y \notin W^{2,p}(\Omega; \mathbb{R}^3) \). To be specific, we choose for \( 1 > \varepsilon > 0 \)

\[
f(x_1) = x_1^{1-\varepsilon} \quad \text{and} \quad g(x_1) = x_1^{1+\varepsilon}.
\]

Hence

\[
f'(x_1) = (1-\varepsilon)x_1^{-\varepsilon}, \quad g'(x_1) = (1+\varepsilon)x_1^\varepsilon,
\]

\[
f''(x_1) = -\varepsilon(1-\varepsilon)x_1^{-1-\varepsilon} \quad \text{and} \quad g''(x_1) = \varepsilon(1+\varepsilon)x_1^{1+\varepsilon}.
\]

Since \( x_2 f''(x_1) \) is not integrable, we have \( \nabla^2 y \notin L^1(\Omega; \mathbb{R}^{3\times 3\times 3}) \) and thus \( y \notin W^{2,1}(\Omega; \mathbb{R}^3) \). We have only \( y \in W^{1,p}(\Omega; \mathbb{R}^3) \cap L^\infty(\Omega; \mathbb{R}^3) \) for every \( 1 \leq p < 1/\varepsilon \). Moreover, direct computation shows that both \( \text{Cof} \nabla y \) and \( \det \nabla y \) lie in \( W^{1,\infty} \). Finally, \( \det \nabla y = x_1^2 > 0 \) and \( (\det \nabla y)^{-s} \in L^1(\Omega) \) for all \( 0 < s < 1/2 \).

Therefore, for any \( r, q \geq 1 \), \( s > 0 \), requiring a deformation \( y : \Omega \to \mathbb{R}^3 \) to satisfy \( \det \nabla y \in W^{1,r}(\Omega) \), \( (\det \nabla y)^{-s} \in L^1(\Omega) \) and \( \text{Cof} \nabla y \in W^{1,q}(\Omega; \mathbb{R}^{3\times 3}) \) is a weaker assumption than \( y \in W^{2,1}(\Omega; \mathbb{R}^3) \).
2 Gradient polyconvexity

We start with a definition of gradient polyconvexity.

**Definition 2.1 (See [7]).** Let \( \Omega \subset \mathbb{R}^3 \) be a bounded open domain. Let \( \hat{W} : \mathbb{R}^{3 \times 3} \times \mathbb{R}^{3 \times 3} \times \mathbb{R}^3 \rightarrow \mathbb{R} \cup \{ +\infty \} \) be a lower semicontinuous function. The functional

\[
J(y) = \int_{\Omega} \hat{W}(\nabla y(x), \nabla\text{Cof} \nabla y(x), \nabla|\text{det} \nabla y(x)|)dx,
\tag{2.1}
\]

defined for any measurable function \( y : \Omega \rightarrow \mathbb{R}^3 \) for which the weak derivatives \( \nabla y, \nabla\text{Cof} \nabla y, \nabla|\text{det} \nabla y| \) exist and are integrable is called gradient polyconvex if the function \( \hat{W}(F,\cdot,\cdot) \) is convex for every \( F \in \mathbb{R}^{3 \times 3} \).

With \( J \) defined as in (2.1) and a functional \( y \mapsto \ell(y) \) expressing the (negative) work of external loads we set

\[
I(y) := J(y) - \ell(y).
\tag{2.2}
\]

Besides convexity properties, the results of weak lower semicontinuity of \( I \) on \( W^{1,p}(\Omega;\mathbb{R}^3) \) (for \( 1 \leq p < +\infty \)) rely on suitable coercivity properties. Here we assume that there are numbers \( p,q,r > 1 \) and \( c,s > 0 \) such that

\[
\hat{W}(F,\Delta_1,\Delta_2) \geq \begin{cases} 
c(|F|^p + |\text{Cof} F|^q + (\text{det} F)^r + (\text{det} F)^{-s} + |\Delta_1|^q + |\Delta_2|^r) & \text{if } \text{det} F > 0, \\
+\infty & \text{otherwise.}
\end{cases}
\tag{2.3}
\]

The following existence result is taken from [7]. For the reader’s convenience, we provide a proof below.

**Proposition 2.1.** Let \( \Omega \subset \mathbb{R}^3 \) be a bounded Lipschitz domain, and let \( \Gamma = \Gamma_0 \cup \Gamma_1 \) be a \( \mathcal{A} \)-measurable partition of \( \Gamma = \partial \Omega \) with the area of \( \Gamma_0 > 0 \). Let further \( -\ell : W^{1,p}(\Omega;\mathbb{R}^3) \rightarrow \mathbb{R} \) be a weakly lower semicontinuous functional satisfying for some \( \bar{C} > 0 \) and \( 1 \leq \bar{p} < p \)

\[
\forall y \in W^{1,p}(\Omega;\mathbb{R}^3) : \quad \ell(y) \leq \bar{C}\|y\|_{W^{1,p}(\Omega;\mathbb{R}^3)}^\bar{p}.
\]

Further let \( J \), as in (2.1), be gradient polyconvex on \( \Omega \) and such that there is a \( \hat{W} \) as in Definition 2.1 which in addition satisfies (2.3) for \( p > 2, \frac{p}{r-1} \leq \bar{p}, r > 1, s > 0 \). Moreover, assume that for some given measurable function \( y_0 : \Gamma_0 \rightarrow \mathbb{R}^3 \) the following set

\[
\mathcal{A} := \{ y \in W^{1,p}(\Omega;\mathbb{R}^3) : \text{Cof} \nabla y \in W^{1,q}(\Omega;\mathbb{R}^{3 \times 3}), \text{det} \nabla y \in W^{1,r}(\Omega), \text{det} \nabla y > 0 \text{ a.e. in } \Omega, y = y_0 \text{ on } \Gamma_0 \}
\]

is nonempty. If \( \inf_{\mathcal{A}} J < \infty \) for \( I \) from (2.2), then the functional \( I \) has a minimizer on \( \mathcal{A} \).

**Proof.** Our proof closely follows the approach in [7]. Let \( \{y_k\} \subset \mathcal{A} \) be a minimizing sequence of \( I \). Due to coercivity assumption (2.3) and the Dirichlet boundary conditions on \( \Gamma_0 \), we obtain that

\[
\sup_{k \in \mathbb{N}} (\|y_k\|_{W^{1,p}(\Omega;\mathbb{R}^3)} + \|\text{Cof} \nabla y_k\|_{W^{1,q}(\Omega;\mathbb{R}^{3 \times 3})} + \|\text{det} \nabla y_k\|_{W^{1,r}(\Omega)} + \|(\text{det} \nabla y_k)^{-s}\|_{L^1(\Omega)}) < \infty.
\tag{2.4}
\]
Hence, by standard results on weak convergence of minors, see e.g. [9, Thm. 7.6-1], there are (non-relabeled) subsequences such that

\[ y_k \rightharpoonup y \text{ in } W^{1,p}(\Omega; \mathbb{R}^3), \quad \text{Cof } \nabla y_k \rightharpoonup \text{Cof } \nabla y \text{ in } L^q(\Omega; \mathbb{R}^{3 \times 3}), \quad \det \nabla y_k \rightharpoonup \det \nabla y \text{ in } L^r(\Omega) \]

for \( k \to \infty \). Moreover, since bounded sets in Sobolev spaces are weakly sequentially compact,

\[ \text{Cof } \nabla y_k \rightharpoonup H \text{ in } W^{1,q}(\Omega; \mathbb{R}^{3 \times 3}), \quad \det \nabla y_k \rightharpoonup D \text{ in } W^{1,r}(\Omega) \] (2.5)

for some \( H \in W^{1,q}(\Omega; \mathbb{R}^{3 \times 3}) \) and \( D \in W^{1,r}(\Omega) \). Since the weak limit is unique, we have \( H = \text{Cof } \nabla y \) and \( D = \det \nabla y \). By compact embedding also \( \text{Cof } \nabla y_k \rightharpoonup H \) in \( W^{1,q}(\Omega; \mathbb{R}^{3 \times 3}) \) and hence we obtain a (non-relabeled) subsequence such that for \( k \to \infty \)

\[ \text{Cof } \nabla y_k \to \text{Cof } \nabla y \text{ a.e. in } \Omega. \] (2.6)

Since by Cramer’s formula \( \det(\text{Cof } \nabla y) = (\det \nabla y)^2 \), we have for \( k \to \infty \)

\[ \det \nabla y_k \to \det \nabla y \text{ a.e. in } \Omega. \] (2.7)

Next we show that \( y \) belongs to the set of admissible functions \( \mathcal{A} \). Notice that \( \det \nabla y_k > 0 \) for any \( k \in \mathbb{N} \). Further, the conditions (2.3), (2.4), and the Fatou lemma imply that

\[ +\infty > \liminf_{k \to \infty} J(y_k) + \ell(y_k) \geq \liminf_{k \to \infty} \int_{\Omega} \frac{1}{(\det \nabla y_k(x))^s} \, dx \geq \int_{\Omega} \frac{1}{(\det \nabla y(x))^s} \, dx. \]

Hence, inevitably, \( \det \nabla y > 0 \) almost everywhere in \( \Omega \) and \( (\det \nabla y)^{-s} \in L^1(\Omega) \). Since the trace operator is continuous, we obtain that \( y \in \mathcal{A} \).

By Cramer’s rule, the inverse of the deformation gradient satisfies for almost all \( x \in \Omega \) that

\[ (\nabla y_k(x))^{-1} = \frac{(\text{Cof } \nabla y_k(x))^\top}{\det \nabla y_k(x)} \to \frac{(\text{Cof } \nabla y(x))^\top}{\det \nabla y(x)} = (\nabla y(x))^{-1}. \] (2.8)

Notice that, for almost all \( x \in \Omega \)

\[ \sup_{k \in \mathbb{N}} |\nabla y_k(x)| = \sup_{k \in \mathbb{N}} \det \nabla y_k(x) \ |(\text{Cof } \nabla y_k(x))^{-\top}| \]

\[ \leq \sup_{k \in \mathbb{N}} \frac{3}{2} \det \nabla y_k(x) \ |(\nabla y_k(x))^{-1}|^2 < \infty \]

because of the pointwise convergence of \( \{\det \nabla y_k\} \) and (2.8). Consequently, we have due to (2.8) for almost all \( x \in \Omega \) and \( k \to \infty \)

\[ \nabla y_k(x) = (\text{Cof } \nabla y_k(x))^{-\top} \det \nabla y_k(x) \to (\text{Cof } \nabla y(x))^{-\top} \det \nabla y(x) = \nabla y(x), \]

where we have used that the cofactor of some matrix is invertible whenever the matrix itself is invertible too. As the Lebesgue measure on \( \Omega \) is finite, we get by the Egoroff theorem, c.f. [14, Thm. 2.22],

\[ \nabla y_k \rightharpoonup \nabla y \text{ in measure.} \] (2.9)
Since \( \hat{W} \) is nonnegative and continuous and \( \hat{W}(F, \cdot, \cdot) \) is convex, we may use [14, Cor. 7.9] to conclude from (2.9) and (2.5) that

\[
\int_\Omega \hat{W}(\nabla y(x), \nabla \text{Cof} \nabla y(x), \nabla \det \nabla y(x)) \, dx \\
\leq \liminf_{k \to \infty} \int_\Omega \hat{W}(\nabla y_k(x), \nabla \text{Cof} \nabla y_k(x), \nabla \det \nabla y_k(x)) \, dx .
\]

To pass to the limit in the functional \(-\ell\), we exploit its weak lower semicontinuity. Therefore, the whole functional \( I \) is weakly lower semicontinuous along \( \{y_k\} \subset \mathcal{A} \) and hence \( y \in \mathcal{A} \) is a minimizer of \( I \).

**Remark 2.2.** Note that the pointwise convergence (2.7) of the determinant, necessary for obtaining the crucial convergence (2.9), was not achieved by compact embedding, as it was done for \( \text{Cof} \nabla y \) in (2.6). Hence the coercivity in \( \nabla[\det \nabla y] \) is of minor importance and can be relaxed, provided the function \( \hat{W} \) from (2.1) does not depend on its last argument, c.f. [7, Prop. 5.1]. On the other hand, although only \( \nabla[\text{Cof} \nabla y] \) is necessary for regularizing the whole problem, making the functional in (2.1) dependent also on \( \nabla[\det \nabla y] \) may be interesting from the applications’ point of view.

Let \( \mathcal{L}^3 \) denote the Lebesgue measure in \( \mathbb{R}^3 \). If \( p > 3 \) and \( y \in W^{1,p}(\Omega; \mathbb{R}^3) \) is such that \( \det \nabla y > 0 \) almost everywhere in \( \Omega \), then the so-called Ciarlet-Nečas condition

\[
\int_\Omega |\nabla y|^3 \, dx \leq \mathcal{L}^3(y(\Omega))
\]

(2.10)

derived in [10] ensures almost-everywhere injectivity of deformations. If

\[
\frac{|\nabla y|^3}{\det \nabla y} \in L^\delta(\Omega)
\]

(2.11)

for some \( \delta > 2 \) and (2.10) holds, then we even get invertibility everywhere in \( \Omega \) due to [17, Theorem 3.4]. Namely, this then implies that \( y \) is an open map. Hence, we get the following corollary of Proposition 2.1.

**Corollary 2.3.** Let \( \Omega \subset \mathbb{R}^3 \) be a bounded Lipschitz domain, and let \( \Gamma = \Gamma_0 \cup \Gamma_1 \) be a \( dA \)-measurable partition of \( \Gamma = \partial \Omega \) with the area of \( \Gamma_0 > 0 \). Let further \( \ell : W^{1,p}(\Omega; \mathbb{R}^3) \to \mathbb{R} \) be a weakly upper semicontinuous functional and \( J \) as in (2.1) be gradient polyconvex on \( \Omega \) such that \( W \) satisfies (2.3). Finally, let \( p > 6, q \geq \frac{6}{p-1}, r > 1, s > 2p/(p-6) \), and assume that for some given measurable function \( y_D : \Gamma_D \to \mathbb{R}^3 \) the following set

\[
\mathcal{A} := \{ y \in W^{1,p}(\Omega; \mathbb{R}^3) : \text{Cof} \nabla y \in W^{1,q}(\Omega; \mathbb{R}^{3 \times 3}), \ \det \nabla y \in W^{1,r}(\Omega), \ \ (\det \nabla y)^{-s} \in L^1(\Omega), \ \det \nabla y > 0 \ a.e. \ in \ \Omega, \ \ y = y_D \ on \ \Gamma_D, \ (2.10) \ holds \}
\]

is nonempty. If \( \inf_{\mathcal{A}} I < \infty \) for \( I \) from (2.2) then the functional \( I \) has a minimizer on \( \mathcal{A} \) which is injective everywhere in \( \Omega \).

A simple example of an energy density which satisfies the assumptions of Proposition 2.3 and Corollary 2.3 is

\[
\hat{W}(F, \Delta_1, \Delta_2) = \begin{cases} 
W(F) + \varepsilon(|F|^p + |\text{Cof} F|^q + (\det F)^r + (\det F)^{-s} + |\Delta_1|^q + |\Delta_2|^r) & \text{if } \det F > 0, \\
+\infty & \text{otherwise}
\end{cases}
\]

for \( W \) defined in (1.5).
Remark 2.4 (Gradient-polyconvex materials and smoothness of stress). Gradient-polyconvex materials enable us to control regularity of the first Piola-Kirchhoff stress tensor by means of smoothness of the Cauchy stress. Assume that the Cauchy stress tensor $T^y : y(\Omega) \rightarrow \mathbb{R}^{3\times 3}$ is Lipschitz continuous, for instance. If $\text{Cof} \nabla y : \Omega \rightarrow \mathbb{R}^{3\times 3}$ is Lipschitz continuous too, then the first Piola-Kirchhoff stress tensor $S$ inherits the Lipschitz continuity from $T^y$ because

$$S(x) := T^y(x^y) \text{Cof} \nabla y(x),$$

where $x^y := y(x)$. In a similar fashion, one can transfer Hölder continuity of $T^y$ to $S$ via Hölder continuity of $x \mapsto \text{Cof} \nabla y$.

In literature, examples of stored energy density functions in nonlinear elasticity are usually minimized on $\text{SO}(3)$. In the context of shape-memory alloys, the stored energy density is minimized on $\text{SO}(3)$ and that $V^i$ is polyconvex, so is $W_i$. Notice also that if $V$ is polyconvex, so is $W_i$.

3 Evolution

If the loading changes in time or if the boundary condition becomes time-dependent, then the specimen evolves as well. Evolution is typically connected with energy dissipation. Experimental evidence shows that considering a rate-independent dissipation mechanism is a reasonable approximation in a wide range of rates of external loads. We hence need to define a suitable dissipation function. Since we consider a rate-independent processes, this dissipation will be positively one-homogeneous. We associate the dissipation to the magnitude of the time derivative of the dissipative variable $z \in \mathbb{R}^{M+1}$, where $M \in \mathbb{N}$, i.e. to $|\dot{z}|_{M+1}$, where $| \cdot |_{M+1}$ denotes a norm on $\mathbb{R}^{M+1}$ (in our setting, the internal variable $z$ can be seen as a vector of volume fractions of austenite and variants of martensite). Therefore, the specific dissipated energy associated to a change from state $z^1$ to $z^2$ is postulated as

$$D(z^1, z^2) := |z^1 - z^2|_{M+1}.$$

Hence, for $z^i : \Omega \rightarrow \mathbb{R}^{M+1}$, $i = 1, 2$, the total dissipation reads

$$D(z^1, z^2) := \int_{\Omega} D(z^1(x), z^2(x)) \, dx,$$

and the total $D$-dissipation of a time dependent curve $z : t \in [0, T] \mapsto z(t)$, where $z(t) : \Omega \rightarrow \mathbb{R}^{M+1}$, is defined as

$$\text{Diss}_D(z[s, t]) := \sup \left\{ \sum_{j=1}^{N} D(z(t_{i-1}), z(t_i)) : N \in \mathbb{N}, s = t_0 \leq \ldots \leq t_N = t \right\}$$

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Let \( Z \) denote the set of all admissible states of internal variable \( s \) \( : \Omega \to \mathbb{R}^{M+1} \) and \( A \) be the set of admissible deformations as before. For a given \((t, y, z) \in [0, T] \times A \times Z\) we define the total energy of the system by

\[
E(t, y, z) = \begin{cases} 
J(y) - L(t, y) & \text{if } z = \lambda(\nabla y) \text{ a.e. in } \Omega, \\
+\infty & \text{otherwise,}
\end{cases}
\]

where \( L(t, \cdot) \) is a functional on deformations expressing time-dependent loading of the specimen and \( \lambda : \mathbb{R}^{3 \times 3} \to \mathbb{R}^{M+1} \) is a function relating the deformation gradient with the internal variable \( z \). For example, we can define the \( j \)th component of \( \lambda \in \mathbb{R}^{M+1} \) as

\[
\lambda_j(F) := \frac{1}{M} \left( 1 - \frac{\text{dist}(C_i, N(C_j))}{\sum_{i=0}^{M} \text{dist}(C, N(C_i))} \right) \quad \forall C = F^T F \in \mathbb{R}^{3 \times 3}, \quad j = 0, \ldots, M,
\]

where \( N(C_i) \) are pairwise disjoint neighborhoods of \( C_i, i = 0, \ldots, M \).

**Remark 3.1.** The particular choice of \( \lambda \) allows for some elastic behavior close to the wells \( SO(3) F_i, i = 0, \ldots, M \). Note that \( \lambda \) is continuous and frame-indifferent, and \( \sum_{j=0}^{M} \lambda_j(F) = 1 \) for all \( F \in \mathbb{R}^{3 \times 3} \).

### 4 Energetic solution

Suppose, that we look for the time evolution of \( t \mapsto y(t) \in A \) and \( t \mapsto z(t) \in Z := L^{\infty}(\Omega, \mathbb{R}^{M+1}) \) during a process on a time interval \([0, T]\), where \( T > 0 \) is the time horizon. We use the following notion of solution from [16], see also [19, 20]. For a given energy \( E \), dissipation distance \( D \) and every admissible configuration living in

\[
Q := \{(y, z) \in A \times Z : \lambda(\nabla y) = z \text{ a.e. in } \Omega\}
\]

we ask the following conditions to be satisfied.

**Definition 4.1 (Energetic solution).** We say that \((y, z) : [0, T] \to Q\) is an energetic solution to \((Q, E, D)\) if \( t \mapsto \partial_t E(y(t), z(t)) \in L^1(0, T) \) and if for all \( t \in [0, T] \) the stability condition

\[
E(t, y(t), z(t)) \leq E(t, \bar{y}, \bar{z}) + D(z(t), \bar{z}) \quad \forall (\bar{y}, \bar{z}) \in Q.
\]

(S)

and the energy balance

\[
E(t, y(t), z(t)) + \text{Diss}_D(z; [s, t]) = E(s, y(s), z(s)) + \int_s^t \partial_s E(s, y(s), z(s)) \, ds
\]

(E)

are satisfied.

An important role is played by the set of so-called stable states, defined for each \( t \in [0, T] \) as

\[
S(t) := \{(y, z) \in Q : E(t, y, z) < +\infty \text{ and } E(t, y, z) \leq E(t, \bar{y}, \bar{z}) + D(z, \bar{z}) \forall (\bar{y}, \bar{z}) \in Q\}.
\]
4.1 Existence of the energetic solution

A standard way how to prove the existence of an energetic solution is to construct time-discrete minimization problems and then to pass to the limit. Before we give the existence proof we need some auxiliary results. For given $N \in \mathbb{N}$ and for $0 \leq k \leq N$, we define the time increments $t_k := kT/N$. Furthermore, we use the abbreviation $q := (y, z) \in Q$. We assume that there exists an admissible deformation $y^0$ compatible with the initial volume fraction $z^0$, i.e. $q^0 := (y^0, z^0) \in \mathbb{S}(0)$. For $k = 1, \ldots, N$, we define a sequence of minimization problems

$$\text{minimize } \mathcal{I}_k(y, z) := \mathcal{E}(t_k, y, z) + \mathcal{D}(z, z^{k-1}), \quad (y, z) \in Q.$$ (4.1)

We denote a minimizer of (4.1) for a given $k$ as $q^k := (y^k, z^k) \in Q$ for $1 \leq k \leq N$. The following lemma shows that a minimizer always exists if the elastic energy is not identically infinite on $\Gamma$.

Lemma 4.1. Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain, and let $\Gamma = \Gamma_0 \cup \Gamma_1$ be a $d\Lambda$-measurable partition of $\Gamma = \partial \Omega$ with the area of $\Gamma_D > 0$. Let $J_k$ of the from (2.1), be gradient polyconvex on $\Omega$ and such that the stored energy density $W$ satisfies (2.3). Moreover, let $L \in C^1([0, T]; W^{1-p}(\Omega; \mathbb{R}^3))$ be such that for some $C > 0$ and $1 \leq \alpha < p$

$$L(t, y) \leq C\|y\|_{W^{1,p}} \quad \forall t \in [0, T]$$

and $y \mapsto -L(t, y)$ be weakly lower semicontinuous on $W^{1,p}(\Omega; \mathbb{R}^3)$ for all $t \in [0, T]$. Finally, let $p > 6$, $q \geq \frac{2}{p-1}$, $r > 1$, $s > 2p/(p - 6)$.

If there is $(y, z) \in Q$ such that $\mathcal{I}_k(y, z) < \infty$ for $\mathcal{I}_k$ from (4.1), then the functional $\mathcal{I}_k$ has a minimizer $q^N_k = (y^k, z^k) \in Q$ such that $y_k$ is injective everywhere in $\Omega$. Moreover, $q^N_k \in \mathbb{S}(t_k)$ for all $1 \leq k \leq N$.

Proof. Since the discretized problem (4.1) has a purely static character, we can follow the proof of Proposition 2.1. Let $\{(y_j^k, z_j^k)\}_{j \in \mathbb{N}} \subset Q$ be a minimizing sequence. As

$$\nabla y_j^k \rightharpoonup \nabla y^k \quad \text{strongly in } L^\rho(\Omega, \mathbb{R}^{3 \times 3}) \text{ as } j \to \infty$$

for every $1 \leq \rho < p$ and $\lambda \in C(\mathbb{R}^{3 \times 3}, \mathbb{R}^{M+1})$ is bounded, we obtain that

$$z_j^k = \lambda(\nabla y_j^k) \rightharpoonup \lambda(\nabla y^k) \quad \text{strongly in } L^\rho(\Omega, \mathbb{R}^{M+1}) \text{ as } j \to \infty.$$ Since $\|z_j^k\|_{L^3(\Omega, \mathbb{R}^{M+1})}$ is uniformly bounded in $j$, there is a subsequence such that $z_j^k \rightarrow \mu^k$ in Radon measures on $\Omega$. This shows that $z^k := \mu^k = \lambda(\nabla y^k)$ and hence $q^N_k = (y^k, z^k) \in Q$. Since $\mathcal{D}(\cdot, z^{k-1})$ is convex, we obtain that $q^N_k$ is indeed a minimizer of $\mathcal{I}_k$. Moreover, $y_k$ is injective everywhere by the reasoning used for proving Corollary 2.3 The stability $q^N_k \in \mathbb{S}(t_k)$ follows by standard arguments, see e.g. [16].

Denoting by $B([0, T]; A)$ the set of bounded maps $t \mapsto y(t) \in A$ for all $t \in [0, T]$, we have the following result showing the existence of an energetic solution to the problem $(Q, \mathcal{E}, \mathcal{D})$.

Theorem 4.1. Let $T > 0$ and let the assumptions in Lemma 4.1 be satisfied. Moreover, let the initial condition be stable, i.e. $q^0 := (y^0, z^0) \in \mathbb{S}(0)$. Then there is an energetic solution to $(Q, \mathcal{E}, \mathcal{D})$ satisfying $q(0) = q^0$ and such that $y \in B([0, T]; A)$, $z \in BV([0, T]; L^1(\Omega; \mathbb{R}^{M+1})) \cap L^\infty(0, T; Z)$, and for all $t \in [0, T]$ the identity $\lambda(\nabla y(t, \cdot)) = z(t, \cdot)$ holds a.e. in $\Omega$. Moreover, for all $t \in [0, T]$ the deformation $y(t)$ is injective everywhere in $\Omega$. 

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Proof. Let \( q^N_k := (y^k, z^k) \) be the solution of (4.1) which exists by Lemma 4.1 and let \( q^N : [0, T] \to Q \) be given by

\[
q^N(t) := \begin{cases} 
q^N_k & \text{if } t \in [t_k, t_{k+1}) \text{ if } k = 0, \ldots, N - 1, \\
q^N_N & \text{if } t = T.
\end{cases}
\]

Following [16], we get for some \( C > 0 \) and for all \( N \in \mathbb{N} \) the estimates

\[
\|z^N\|_{BV(0,T; L^1(\Omega; \mathbb{R}^{M+1}))} \leq C, \quad \|z^N\|_{L^\infty(0,T; BV(\Omega; \mathbb{R}^{M+1}))} \leq C, \quad (4.2a)
\]

\[
\|y^N\|_{L^\infty(0,T; W^{1,p}(\Omega; \mathbb{R}^3))} \leq C, \quad (4.2b)
\]

as well as the following two-sided energy inequality

\[
\int_{t_{k-1}}^{t_k} \partial_t \mathcal{E}(\theta, q^N_k) \, d\theta \leq \mathcal{E}(t_k, q^N_k) + D(z^k, z^{k-1}) - \mathcal{E}(t_{k-1}, q^N_{k-1}) \\
\leq \int_{t_{k-1}}^{t_k} \partial_t \mathcal{E}(\theta, q^N_k) \, d\theta. \quad (4.3)
\]

The second inequality in (4.3) follows since \( q^N_k \) is a minimizer of (4.1) and by comparison of its energy with \( q := q^N_{k-1} \). The lower estimate is implied by the stability of \( q^N_{k-1} \in S(t_{k-1}) \), see Lemma 4.1 when compared with \( \tilde{q} := q^N_k \). Having this inequality, the a-priori estimates and a generalized Helly’s selection principle [20, Cor. 2.8], we get that there is indeed an energetic solution obtained as a limit for \( N \to \infty \).

Let us comment more on the two main properties of the minimizer, namely that it is orientation preserving and injective everywhere in \( \Omega \). The condition \( \det \nabla y > 0 \) a.e. in \( \Omega \) follows from the fact that if \( t_j \to t \), \((y(j), z(j)) \in S(t_j)\) and \((y(j), z(j)) \rightharpoonup (y, z) \in W^{1,p}(\Omega; \mathbb{R}^3) \times BV(\Omega; \mathbb{R}^{M+1})\), then \((y, z) \in S(t)\). Indeed, we have \( z(j) \to z \) in \( L^1(\Omega; \mathbb{R}^{M+1}) \) in our setting and hence for all \((\tilde{y}, \tilde{z}) \in Q \), we get

\[
\mathcal{E}(t, y, z) \leq \liminf_{j \to \infty} \mathcal{E}(t_j, y(j), z(j)) \leq \liminf_{j \to \infty} (\mathcal{E}(t_j, \tilde{y}, \tilde{z}) + D(z(j), \tilde{z})) \\
= \mathcal{E}(t, \tilde{y}, \tilde{z}) + D(z, \tilde{z}).
\]

In particular, as \( \mathcal{E}(t_j, \tilde{y}, \tilde{z}) \) is finite for some \((\tilde{y}, \tilde{z}) \in Q \), we get \( \mathcal{E}(t, y, z) < +\infty \) and thus \( \nabla y > 0 \) a.e. in \( \Omega \) in view of (2.3).

In proving injectivity, we profit again from the fact that quasistatic evolution of energetic solutions is very close to a purely static problem. In view of (4.2b), we obtain for each \( t \in [0, T] \) all necessary convergences that were used in the proof of Corollary 2.3 to pass to the limit in the conditions (2.10) and (2.11).

\[\square\]

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