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Gradient Polyconvexity in Evolutionary Models of Shape-Memory Alloys

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Abstract

We show the 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 the existence of a solution based on weak continuity of nonlinear minors of deformation gradients in Sobolev spaces. Admissible deformations do not necessarily have integrable second derivatives. Under suitable assumptions, our model allows for solutions which are orientation preserving and globally injective everywhere in the domain representing the specimen.

Keywords Gradient polyconvexity · Invertibility of deformations · Orientation-preserving mappings · Shape-memory alloys

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1 Introduction

The idea of non-simple materials can be traced back to 1901 when Korteweg considered a gradient of the density in his model of fluid capillarity. Considering more than only the first deformation gradient in the description of elastic behavior of solids goes back to the 1960s and appeared in the work of Toupin [1,2], and Green and Rivlin [3], such materials are usually called N-grade materials, where N refers to the highest deformation gradient appearing in the model. This approach has brought questions on thermodynamical consistency of such models, treated in [4,5], for instance. From then on, it has been used in many works, see, e.g., [6–12]. Mathematically, the presence of higher-order gradients in the model brings additional compactness properties for the set of admissible functions and ensures the existence of minimizers. We refer to recent related results on the mathematical treatment of shape-memory materials: [13,14]. We also refer to [15] for an overview.

The aim of this contribution is to apply a new class of non-simple material models introduced in [16] (called *gradient polyconvex materials*) to evolutionary problems of shape-memory alloys. The novelty consists in considering only gradients on nonlinear minors in the stored energy density of the material. It is shown there, and also in Example 2.1, that corresponding deformations do not necessarily have integrable second weak derivatives. Nevertheless, it is possible to prove the existence of an energetic solution. The plan of the paper is as follows: We first introduce necessary notation and tools in Sect. 2. The notion of gradient polyconvexity is thoroughly discussed in Sect. 3 and the quasistatic evolution in Sect. 4. Finally, we close our exposition with a short conclusion.

2 Preliminaries

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,

$$S := \frac{\partial W(F)}{\partial F} \tag{1}$$

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 $R \in \mathrm{SO}(3)$,

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

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

$$W(F) \to +\infty, \quad \text{if } \det F \searrow 0. \tag{2}$$

Let the reference configuration be a bounded Lipschitz domain $\Omega \subset \mathbb{R}^3$. Deformation $y : \bar{\Omega} \to \mathbb{R}^3$ maps the points in the closure of the reference configuration $\bar{\Omega}$ to their positions in the deformation configuration. Solutions to the corresponding elasticity equations can then be formally found by minimizing the energy functional

$$I(y) := \int_\Omega W(\nabla y(x))\,\mathrm{d}x - \ell(y) \tag{3}$$

over the class of admissible deformations. Here, ℓ is a functional on the set of deformations, expressing (in a simplified way) the work of external loads on the specimen, and ∇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 $(Fa \times Fb) \cdot Fc > 0$ 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 on matrices with non-positive determinants, i.e.,

$$W(F) := +\infty, \quad \text{if } \det F \leq 0. \tag{4}$$

In view of (1), (2), and (4), we see that $W : \mathbb{R}^{3\times 3} \to [-w, +\infty]$ is continuous in the sense that if $F_k \to F$ in $\mathbb{R}^{3\times 3}$ 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 (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 to a discussion of the assumptions on W. It is well known that (2) prevents us from assuming convexity of W. See, for example, [17] or the recent review for a detailed exposition of weak lower semicontinuity. Following earlier work by C. B. Morrey, Jr., [18], J. M. Ball [19] defined a polyconvex stored energy density W by assuming that there is a convex and lower semicontinuous function $\overline{W} : \mathbb{R}^{19} \to [-w, +\infty]$ such that

$$W(F) := \overline{W}(F, \operatorname{Cof} F, \det F) \quad \forall F \in \mathbb{R}^{3\times 3}.$$

Here, $\operatorname{Cof} F$ denotes the cofactor matrix of F, which, for F being invertible, satisfies Cramer's rule:

$$\operatorname{Cof} F = (\det F)(F^{-1})^\top.$$

It is well known that polyconvexity is satisfied for a large class of constitutive functions and allows for the existence of minimizers of I under (2) and (4). On the other hand, there are still situations where polyconvexity cannot be adopted. A prominent example is shape-memory alloy, where W has the so-called multi-well structure, see, for example, [20–22]. 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, for example, in three for the tetragonal structure (NiMnGa) or in twelve for the monoclinic one (NiTi). We can assume that

$$W(F) := \min_{0 \le i \le M} W_i(F), \tag{5}$$

where $W_i : \mathbb{R}^{3\times 3} \to [-w_i, +\infty]$, $w_i \ge 0$, 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, we have $W_i(F) = -w_i$ if and only if $F = RF_i$ for a given matrix $F_i \in \mathbb{R}^{3\times 3}$ and an arbitrary proper rotation $R \in \mathrm{SO}(3)$. This means that each variant of the martensite and the austenite is modeled as a hyperelastic material with its own stored energy density W_i. We also assume that each W_i is differentiable on the set of matrices with positive determinants. Thus, the variants can be described independently, e.g., the elastic constants can be chosen differently. The drawback is obviously the non-smoothness of W; however, physically realistic elastic strain values do not occur in the set where W is not differentiable. We refer, for example, to [23] for other models of the stored energy density of shape-memory alloys.

Given a deformation gradient F, we need to decide whether the corresponding deformation is in the well of the austenite, or in a martensitic variant. In order to do so, we define a volume fraction $\lambda(F)$ as follows:

Let $\lambda : \mathbb{R}^{3\times 3} \to \mathbb{R}^{M+1}$. Set

$$\lambda^j(F) := \frac{1}{M}\left(1 - \frac{\mathrm{dist}(C, \mathcal{N}(C_j))}{\sum_{i=0}^{M} \mathrm{dist}(C, \mathcal{N}(C_i))}\right) \quad \forall C = F^T F \in \mathbb{R}^{3\times 3}, \quad j = 0, \ldots, M, \tag{6}$$

where $\mathcal{N}(C_i)$ are pairwise disjoint neighborhoods of the strain tensors $C_i = F_i^\top F_i$, for $i \in \{0, \ldots, M\}$. Notice that $\sum_{i=0}^{M} \lambda^j(F) = 1$ for every F, which, together with $\lambda^j > 0$, allows us to interpret λ as a volume fraction. Moreover, note that λ is continuous and frame indifferent in the sense that $\lambda(F) = \lambda(RF)$ for every proper rotation R. Volume fractions will play an important role in the definition of our evolutionary model in Sect. 4.

Remark 2.1 Note that this particular choice of λ allows for some elastic behavior close to the wells $SO(3)F_i, i = 0, \ldots, M$, since the volume fraction remains constant on the neighborhoods $\mathcal{N}(C_i)$, $i = 0, \ldots, M$.

Let us emphasize that (5) ruins even generalized notions of convexity as, for example, rank-one convexity. (We recall that rank-one convex functions are convex on the line segments with endpoints differing by a rank-one matrix and that rank-one convexity is a necessary condition for polyconvexity; cf. [17], for instance.) Namely, it is observed (see, e.g., [20,21]) that $w_i = w_j$, whenever $i, j \ne 0$, and that there is a proper rotation R_{ij} such that $\mathrm{rank}(R_{ij}F_i - F_j) = 1$. 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. Nevertheless, 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. This is mathematically manifested via a 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., [17]. Such a relaxation yields information of the effective behavior 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. This in particular implies that $W < +\infty$. We refer, however, to [24–26] for results allowing for infinite energies. Nevertheless, these works include other assumptions that severely restrict their usage. Let us point out that the right Cauchy–Green strain tensor $F^\top F$ maps $\mathrm{SO}(3)F$ as well as $(\mathrm{O}(3)\setminus\mathrm{SO}(3))F$ to the same point. Here, $\mathrm{O}(3)$ are the orthogonal matrices with determinant ± 1. Thus, for example, $F \mapsto |F^\top F - \mathbb{I}|$ is minimized on two energy wells, on $\mathrm{SO}(3)$ and also on $\mathrm{O}(3)\setminus\mathrm{SO}(3)$. 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 also on higher-order derivatives. Simple examples are functionals of the form

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

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

$$\nabla y \mapsto \int_\Omega W(\nabla y(x)) \,\mathrm{d}x$$

for existence of minimizers.

Here, we follow a different approach, recently suggested in [16], 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 density of the material depends on the deformation gradient ∇y and on gradients of nonlinear minors of ∇y, i.e., on $\nabla[\mathrm{Cof}\,\nabla y]$ 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 variables, this is not assumed in the ∇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 [16]. It shows that there are maps with smooth nonlinear minors whose deformation gradient is *not* a Sobolev map. Hence, gradient polyconvex energies are more general than second gradient ones.

Example 2.1 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,

$$\nabla y(x_1, x_2, x_3) = \begin{pmatrix} 1 & 0 & 0 \\ x_2 f'(x_1) & f(x_1) & 0 \\ x_3 g'(x_1) & 0 & g(x_1) \end{pmatrix},$$
$$\mathrm{Cof}\nabla y(x_1, x_2, x_3) = \begin{pmatrix} f(x_1)g(x_1) & -x_2 f'(x_1)g(x_1) & -x_3 f(x_1)g'(x_1) \\ 0 & g(x_1) & 0 \\ 0 & 0 & f(x_1) \end{pmatrix}$$

and

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

Finally, the nonzero entries of $\nabla^2 y(x_1, x_2, x_3)$ are

$$x_2 f''(x_1), \quad f'(x_1), \quad x_3 g''(x_1), \quad g'(x_1). \tag{7}$$

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 $y \in W^{1,p}(\Omega; \mathbb{R}^3)$, $\mathrm{Cof}\nabla y \in W^{1,q}(\Omega; \mathbb{R}^{3\times 3})$, $0 < \det \nabla y \in W^{1,r}(\Omega)$, $(\det \nabla y)^{-s} \in L^1(\Omega)$ for some $p, q, r \geq 1$ and $s > 0$, but such that one of the quantities in (7) is 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,

$$f'(x_1) = (1-\varepsilon)x_1^{-\varepsilon}, \qquad g'(x_1) = (1+\varepsilon)x_1^{\varepsilon},$$
$$f''(x_1) = -\varepsilon(1-\varepsilon)x_1^{-1-\varepsilon}, \qquad g''(x_1) = \varepsilon(1+\varepsilon)x_1^{-1+\varepsilon}.$$

Since $x_2 f''(x_1)$ is not integrable, we have $\nabla^2 y \notin L^1(\Omega; \mathbb{R}^{3\times3\times3})$, 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 $\mathrm{Cof}\nabla y$ 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 $\mathrm{Cof}\nabla y \in W^{1,q}(\Omega; \mathbb{R}^{3\times3})$ is a weaker assumption than $y \in W^{2,1}(\Omega; \mathbb{R}^3)$.

3 Gradient Polyconvexity

We start with a definition of gradient polyconvexity.

Definition 3.1 (*See* [16]) Let $\hat{W} : \mathbb{R}^{3\times3} \times \mathbb{R}^{3\times3\times3} \times \mathbb{R}^3 \to \mathbb{R} \cup \{+\infty\}$ be a lower semicontinuous function, and let $\Omega \subset \mathbb{R}^3$ be a bounded open domain. The functional

$$J(y) = \int_\Omega \hat{W}(\nabla y(x), \nabla[\mathrm{Cof}\nabla y(x)], \nabla[\det \nabla y(x)])\mathrm{d}x, \tag{8}$$

defined for any measurable function $y : \Omega \to \mathbb{R}^3$ for which the weak derivatives ∇y, $\nabla[\mathrm{Cof}\nabla y]$, $\nabla[\det \nabla y]$ exist and which are integrable, is called *gradient polyconvex* if the function $\hat{W}(F, \cdot, \cdot)$ is convex for every $F \in \mathbb{R}^{3\times3}$.

With J defined as in (8) and a functional $y \mapsto -\ell(y)$ expressing the work of external loads, we set

$$I(y) := J(y) - \ell(y). \tag{9}$$

Besides convexity properties, the results of weak lower semicontinuity of I on $W^{1,p}(\Omega; \mathbb{R}^3)$, in the case $1 \leq p < +\infty$, rely on suitable coercivity properties. Here we assume that there are numbers $q, r > 1$ and $c, s > 0$ such that for every $F \in \mathbb{R}^{3\times3}$, $\Delta_1 \in \mathbb{R}^{3\times3\times3}$, and every $\Delta_2 \in \mathbb{R}^3$

$$\hat{W}(F, \Delta_1, \Delta_2) \geq \begin{cases} c\big(|F|^p + |\mathrm{Cof}\,F|^q + (\det F)^r + (\det F)^{-s} + |\Delta_1|^q + |\Delta_2|^r\big), & \text{if } \det F > 0, \\ +\infty, & \text{otherwise.} \end{cases} \tag{10}$$

The following existence result is taken from [16]. For the reader's convenience, we provide a proof below.

Proposition 3.1 *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain, and let $\Gamma = \Gamma_0 \cup \Gamma_1$ be an $\mathcal{H}^2$-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 lower semicontinuous functional satisfying, for some $\tilde{C} > 0$ and $1 \leq \bar{p} < p$,*

$$\ell(y) \leq \tilde{C}\|y\|^{\bar{p}}_{W^{1,p}(\Omega;\mathbb{R}^3)}, \qquad \textit{for all } y \in W^{1,p}(\Omega; \mathbb{R}^3). \tag{11}$$

Further, let J, as in (8), be gradient polyconvex on Ω and such that there is a $\hat{W}$ as in Definition 3.1 which in addition satisfies (10) for $p > 2$, $q \geq \frac{p}{p-1}$, $r > 1$, $s > 0$. Moreover, assume that, for some given measurable function $y_0 : \Gamma_0 \to \mathbb{R}^3$, the following set

$$\mathcal{A} := \big\{ y \in W^{1,p}(\Omega;\mathbb{R}^3) :\ \mathrm{Cof}\nabla y \in W^{1,q}(\Omega;\mathbb{R}^{3\times 3}),\ \det\nabla y \in W^{1,r}(\Omega), \\ (\det\nabla y)^{-s} \in L^1(\Omega),\ \det\nabla y > 0 \textit{ a.e. in } \Omega,\ y = y_0 \textit{ on } \Gamma_0 \big\}$$

is non-empty. If $\inf_{\mathcal{A}} I < \infty$ for I from (9), then the functional I has a minimizer on $\mathcal{A}$.

Proof Our proof closely follows the approach in [16]. Let $\{y_k\} \subset \mathcal{A}$ be a minimizing sequence of I. Due to coercivity assumption (10), the bound on the loading (11), the Poincaré inequality, and the Dirichlet boundary conditions on Γ_0, we obtain that

$$\sup_{k\in\mathbb{N}} \big(\|y_k\|_{W^{1,p}(\Omega;\mathbb{R}^3)} + \|\mathrm{Cof}\nabla y_k\|_{W^{1,q}(\Omega;\mathbb{R}^{3\times 3})} \\ + \|\det\nabla y_k\|_{W^{1,r}(\Omega)} + \|(\det\nabla y_k)^{-s}\|_{L^1(\Omega)} \big) < \infty. \tag{12}$$

Hence, by standard results on weak convergence of minors, see, e.g., [27, Thm. 7.6-1], there are (not explicitly labeled) subsequences such that

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

for $k \to \infty$. Moreover, since bounded sets in uniformly convex Sobolev spaces are weakly sequentially compact,

$$\mathrm{Cof}\nabla y_k \rightharpoonup H \text{ in } W^{1,q}(\Omega;\mathbb{R}^{3\times 3}), \quad \det\nabla y_k \rightharpoonup D \text{ in } W^{1,r}(\Omega) \tag{13}$$

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 $H = \mathrm{Cof}\nabla y$ and $D = \det\nabla y$. By compact embedding, also $\mathrm{Cof}\nabla y_k \to H$ in $L^q(\Omega;\mathbb{R}^{3\times 3})$ and hence we obtain a (not explicitly labeled) subsequence such that, for $k \to \infty$,

$$\mathrm{Cof}\nabla y_k \to \mathrm{Cof}\nabla y \quad \text{a.e. in } \Omega. \tag{14}$$

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

$$\det\nabla y_k \to \det\nabla y \quad \text{a.e. in } \Omega. \tag{15}$$

Next we show that y belongs to the set of admissible functions $\mathcal{A}$. Notice that $\det\nabla y \geq 0$ since $\det\nabla y_k > 0$ for any $k \in \mathbb{N}$. Further, conditions (10), (11), (12), and the Fatou lemma imply that

$$+\infty > \liminf_{k\to\infty} I(y_k) + \ell(y_k) \geq \liminf_{k\to\infty} \int_\Omega \frac{1}{(\det \nabla y_k(x))^s}\,\mathrm{d}x \geq \int_\Omega \frac{1}{(\det \nabla y(x))^s}\,\mathrm{d}x.$$

Hence, inevitably, $\det \nabla y > 0$ almost everywhere in Ω 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 $x \in \Omega$ and $k \to \infty$, that

$$(\nabla y_k(x))^{-1} = \frac{(\mathrm{Cof}\nabla y_k(x))^\top}{\det \nabla y_k(x)} \longrightarrow \frac{(\mathrm{Cof}\nabla y(x))^\top}{\det \nabla y(x)} = (\nabla y(x))^{-1}. \tag{16}$$

Notice that, for almost all $x \in \Omega$,

$$\begin{aligned}\sup_{k\in\mathbb{N}} |\nabla y_k(x)| &= \sup_{k\in\mathbb{N}} \det \nabla y_k(x)\ |((\mathrm{Cof}(\nabla y_k(x)))^{-1}))^\top| \\ &\leq \sup_{k\in\mathbb{N}} \frac{3}{2} \det \nabla y_k(x)\ |(\nabla y_k(x))^{-1}|^2 < \infty\end{aligned}$$

because of the pointwise convergence of $\{\det \nabla y_k\}$ and (16).

Due to (16), we have, for almost all $x \in \Omega$ and $k \to \infty$, that

$$\begin{aligned}\nabla y_k(x) &= ((\mathrm{Cof}(\nabla y_k(x))^{-1})^\top \det \nabla y_k(x) \longrightarrow ((\mathrm{Cof}(\nabla y(x))^{-1})^\top \det \nabla y(x) \\ &= \nabla y(x),\end{aligned}$$

where we have used that the cofactor of some matrix is invertible whenever the matrix itself is invertible too. As the Lebesgue measure on Ω is finite, we get by the Egoroff theorem, c.f. [28, Thm. 2.22],

$$\nabla y_k \to \nabla y \ \text{ in measure.} \tag{17}$$

Since $\hat{W}$ is nonnegative and continuous and $\hat{W}(F, \cdot, \cdot)$ is convex, we may use [28, Cor. 7.9] to conclude, from (17) and (13), that

$$\begin{aligned}&\int_\Omega \hat{W}(\nabla y(x), \nabla \mathrm{Cof}\nabla y(x), \nabla \det \nabla y(x))\,\mathrm{d}x \\ &\leq \liminf_{k\to\infty} \int_\Omega \hat{W}(\nabla y_k(x), \nabla \mathrm{Cof}\nabla y_k(x), \nabla \det \nabla y_k(x))\,\mathrm{d}x\ .\end{aligned}$$

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 3.1 Note that the pointwise convergence (15) of the determinant, necessary for obtaining the crucial convergence in (17), was not achieved by compact embedding, as it was done for $\operatorname{Cof}\nabla y$ in (14). Hence, the coercivity in $\nabla[\det\nabla y]$ is of minor importance and can be relaxed, provided the function $\hat{W}$ from (8) does not depend on its last argument, c.f. [16, Prop. 5.1]. On the other hand, although only $\nabla[\operatorname{Cof}\nabla y]$ is necessary for regularizing the whole problem, making the functional in (8) 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 Ω, then the so-called Ciarlet–Nečas condition

$$\int_\Omega \det\nabla y(x)\,\mathrm{d}x \le \mathcal{L}^3(y(\Omega)), \tag{18}$$

derived in [29] ensures almost-everywhere injectivity of deformations. We also refer to [30, Sec. 6, Thm.2] and to [31] for other conditions ensuring injectivity of deformations, requiring, however, a prescribed Dirichlet boundary datum on the whole $\partial\Omega$, which is difficult to ensure in a physical laboratory. If

$$\frac{|\nabla y|^3}{\det\nabla y}\in L^\delta(\Omega) \tag{19}$$

for some $\delta>2$ and (18) holds, then we even get invertibility everywhere in Ω due to [32, Theorem 3.4]. Namely, this then implies that y is an open map. Hence, we get the following corollary of Proposition 3.1.

Corollary 3.1 *Let $\Omega\subset\mathbb{R}^3$ be a bounded Lipschitz domain, and let $\Gamma=\Gamma_0\cup\Gamma_1$ be an $\mathcal{H}^2$-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 (8) be gradient polyconvex on Ω such that $\hat{W}$ satisfies (10). Finally, let $p>6$, $q\ge\frac{p}{p-1}$, $r>1$, $s>2p/(p-6)$, and assume that, for some given measurable function $y_0:\Gamma_0\to\mathbb{R}^3$, the following set*

$$\begin{aligned}\mathcal{A}:=\{y\in W^{1,p}(\Omega;\mathbb{R}^3):\ &\operatorname{Cof}\nabla y\in W^{1,q}(\Omega;\mathbb{R}^{3\times3}),\ \det\nabla y\in W^{1,r}(\Omega),\\ &(\det\nabla y)^{-s}\in L^1(\Omega),\ \det\nabla y>0 \textit{ a.e. in } \Omega,\ y=y_0 \textit{ on } \Gamma_0,\ (18) \textit{holds}\}\end{aligned}$$

is non-empty. If $\inf_{\mathcal{A}} I<\infty$ for I from (9), then the functional I has a minimizer on $\mathcal{A}$ which is injective everywhere in Ω.

A simple example of an energy density which satisfies the assumptions of Proposition 3.1 and Corollary 3.1 is

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

for W defined in (5).

Remark 3.2 (**Gradient polyconvex materials and smoothness of stress**) Gradient polyconvex materials enable us to control the regularity of the first Piola–Kirchhoff stress tensor by means of smoothness of the Cauchy stress. Assume that the Cauchy stress tensor $T^y : y(\Omega) \to \mathbb{R}^{3\times 3}$ is Lipschitz continuous, for instance. If $\mathrm{Cof}\nabla y : \Omega \to \mathbb{R}^{3\times 3}$ is Lipschitz continuous too, then the first Piola–Kirchhoff stress tensor S inherits the Lipschitz continuity from T^y because

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

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

In the literature, examples of stored energy density functions in nonlinear elasticity are usually minimized on SO(3). In the context of shape-memory alloys, the stored energy density is minimized on $\mathrm{SO}(3)F_i$, $F_i \neq F_j, i, j = 0, \ldots, M$. To construct such energy densities explicitly, we can now proceed as follows. Assume that $V : \mathbb{R}^{3\times 3} \to \mathbb{R} \cup \{+\infty\}$ is minimized on SO(3) and that $V(F) = \varphi(F^\top F) = \varphi(C)$ for some function $\varphi : \mathbb{R}^{3\times 3}_{sym} \to \mathbb{R} \cup \{+\infty\}$ and the right Cauchy–Green tensor $C = F^\top F$. It is easy to see that φ attains its minimum at the identity matrix $\mathbb{I}$. Considering the polar decomposition of $F_i \in \mathbb{R}^{3\times 3}$ with $\det F_i > 0$, we can write $F_i = R_i U_i$, where R_i is a rotation and U_i is symmetric and positive definite matrix. Note that $C_i := F_i^\top F_i = U_i^2$. Bearing this in mind, we define the energy of the i-th variant via a shift

$$W_i(F) := V\left(FU_i^{-1}\right) = \varphi\left(U_i^{-1}CU_i^{-1}\right),$$

which is clearly minimized on $\mathrm{SO}(3)F_i$. Notice also that if V is polyconvex, so is W_i.

4 Evolution

If the loading changes in time or if the boundary condition becomes time dependent, then the specimen evolves as well. We consider here the case, in which evolution is 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 with the magnitude of the time derivative of the dissipative variable $z \in \mathbb{R}^{M+1}$, where $M \in \mathbb{N}$, i.e., with $|\dot{z}|_{M+1}$, 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 M variants of martensite.) Therefore, the specific dissipated energy associated with a change from state z^1 to z^2 is postulated as

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

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

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

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

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

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

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

where $L(t, \cdot)$ is a functional on deformations expressing time-dependent loading of the specimen, and λ is defined in (6).

4.1 Energetic Solution

Suppose that we look for the time evolution of $t \mapsto y(t) \in \mathcal{A}$ and $t \mapsto z(t) \in \mathcal{Z} := L^\infty(\Omega, \mathbb{R}^{M+1})$ during a process on a time interval $[0, T]$, where $T > 0$ is the time horizon. We use the following notion of solution from [33], see also [34,35].

Definition 4.1 (*Energetic solution*) Let an energy $\mathcal{E} : [0, T] \times \mathcal{A} \times \mathcal{Z} \to \mathbb{R} \cup \{+\infty\}$ and a dissipation distance $\mathcal{D} : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R} \cup \{+\infty\}$ be given. The set of admissible configurations is defined as

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

We say that $(y, z) : [0, T] \to \mathcal{Q}$ is an energetic solution to $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$, if the mapping $t \mapsto \partial_t \mathcal{E}(y(t), z(t))$ is in $L^1(0, T)$ and if, for all $t \in [0, T]$, the stability condition

$$\mathcal{E}(t, y(t), z(t)) \leq \mathcal{E}(t, \tilde{y}, \tilde{z}) + \mathcal{D}(z(t), \tilde{z}) \qquad \forall (\tilde{y}, \tilde{z}) \in \mathcal{Q}. \tag{S}$$

and the energy balance

$$\mathcal{E}(t, y(t), z(t)) + \mathrm{Diss}_{\mathcal{D}}(z; [s, t]) = \mathcal{E}(s, y(s), z(s)) + \int_s^t \partial_t \mathcal{E}(\vartheta, y(\vartheta), z(\vartheta))\, \mathrm{d}\vartheta \tag{E}$$

are satisfied for any $0 \leq s < t \leq T$.

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

$$\mathbb{S}(t) := \{(y, z) \in \mathcal{Q} : \mathcal{E}(t, y, z) < +\infty \text{ and } \mathcal{E}(t, y, z) \le \mathcal{E}(t, \tilde{y}, \tilde{z}) \\ +\mathcal{D}(z, \tilde{z}) \ \ \forall (\tilde{y}, \tilde{z}) \in \mathcal{Q}\}.$$

4.2 Existence of an 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 $0 \le k \le N$, we define the time increments $t_k := kT/N$. Furthermore, we use the abbreviation $q := (y, z) \in \mathcal{Q}$. We assume that there exists an admissible deformation y^0 being 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

$$\text{minimize } \mathcal{I}_k(y, z) := \mathcal{E}(t_k, y, z) + \mathcal{D}\left(z, z^{k-1}\right), \quad (y, z) \in \mathcal{Q}. \tag{20}$$

We denote a minimizer of (20), for a given k, as $q_k^N := (y^k, z^k) \in \mathcal{Q}$ for $1 \le k \le N$. The following lemma shows that a minimizer always exists if the elastic energy is not identically infinite on $\mathcal{Q}$:

Lemma 4.1 *Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain, and let $\Gamma = \Gamma_0 \cup \Gamma_1$ be an $\mathcal{H}^2$-measurable partition of $\Gamma = \partial\Omega$ with the area of $\Gamma_0 > 0$. Let J, of the from (8), be gradient polyconvex on Ω and such that the stored energy density $\hat{W}$ satisfies (10). Moreover, let $L \in C^1([0, T]; W^{1,p}(\Omega; \mathbb{R}^3))$ be such that, for some $C > 0$ and $1 \le \alpha < p$,*

$$L(t, y) \le C\|y\|^{\alpha}_{W^{1,p}}, \quad \textit{for all } t \in [0, T]$$

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

If there is $(y, z) \in \mathcal{Q}$ such that $\mathcal{I}_k(y, z) < \infty$ for $\mathcal{I}_k$ from (20), then the functional $\mathcal{I}_k$ has a minimizer $q_k^N = (y^k, z^k) \in \mathcal{Q}$ such that y_k is injective everywhere in Ω. Moreover, $q_k^N \in \mathbb{S}(t_k)$ for all $1 \le k \le N$.

Proof Since the discretized problem (20) has a purely static character, we can follow the proof of Proposition 3.1. Let $\{(y_j^k, z_j^k)\}_{j\in\mathbb{N}} \subset \mathcal{Q}$ be a minimizing sequence. As

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

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

$$z_j^k = \lambda(\nabla y_j^k) \longrightarrow \lambda(\nabla y^k) \quad \text{strongly in } L^{\tilde{p}}(\Omega, \mathbb{R}^{M+1}) \text{ as } j \to \infty.$$

Since $\|z_j^k\|_{L^1(\Omega,\mathbb{R}^{M+1})}$ is uniformly bounded in j, there is a subsequence (not explicitly relabeled) such that $z_j^k \overset{*}{\rightharpoonup} \mu^k$ in Radon measures on Ω. This shows that $z^k := \mu^k = \lambda(\nabla y^k)$ and hence $q_k^N = (y^k, z^k) \in \mathcal{Q}$. Since $\mathcal{D}(\cdot, z^{k-1})$ is convex, we obtain that q_k^N is indeed a minimizer of $\mathcal{I}_k$. Moreover, y_k is injective everywhere by the reasoning used for proving Corollary 3.1. The stability $q_k^N \in \mathbb{S}(t_k)$ follows by standard arguments; see, e.g., [33]. □

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

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 $(\mathcal{Q}, \mathcal{E}, \mathcal{D})$ satisfying $q(0) = q^0$ and such that $y \in B\,([0,T];\mathcal{A})$, $z \in \mathrm{BV}\left([0,T]; L^1(\Omega;\mathbb{R}^{M+1})\right) \cap L^\infty(0,T;\mathcal{Z})$, and such that for all $t \in [0,T]$ the identity $\lambda(\nabla y(t,\cdot)) = z(t,\cdot)$ holds a.e. in Ω. Moreover, for all $t \in [0,T]$, the deformation $y(t)$ is injective everywhere in Ω.*

Proof Let $q_k^N := (y^k, z^k)$ be the solution of (20), which exists by Lemma 4.1, and let $q^N : [0,T] \to \mathcal{Q}$ be given by

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

Following [33], we get, for some $C > 0$ and for all $N \in \mathbb{N}$, the estimates

$$\|z^N\|_{BV(0,T;L^1(\Omega;\mathbb{R}^{M+1}))} \le C, \qquad \|z^N\|_{L^\infty(0,T;BV(\Omega;\mathbb{R}^{M+1}))} \le C, \tag{21a}$$

$$\|y^N\|_{L^\infty(0,T;W^{1,p}(\Omega;\mathbb{R}^3))} \le C, \tag{21b}$$

as well as the following two-sided energy inequality

$$\begin{aligned} \int_{t_{k-1}}^{t_k} \partial_t \mathcal{E}\left(\theta, q_k^N\right) \mathrm{d}\theta &\le \mathcal{E}\left(t_k, q_k^N\right) + \mathcal{D}\left(z^k, z^{k-1}\right) - \mathcal{E}\left(t_{k-1}, q_{k-1}^N\right) \\ &\le \int_{t_{k-1}}^{t_k} \partial_t \mathcal{E}\left(\theta, q_{k-1}^N\right) \mathrm{d}\theta. \end{aligned} \tag{22}$$

The second inequality in (22) follows since q_k^N is a minimizer of (20) and by comparison of its energy with $q := q_{k-1}^N$. The lower estimate is implied by the stability of $q_{k-1}^N \in \mathbb{S}(t_{k-1})$, see Lemma 4.1, when compared with $\tilde{q} := q_k^N$. By this inequality, the a priori estimates and a generalized Helly's selection principle [35, 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 Ω. The condition $\det \nabla y > 0$ a.e. in Ω follows from the fact that if $t_j \to t$, $(y_{(j)}, z_{(j)}) \in \mathbb{S}(t_j)$ and $(y_{(j)}, z_{(j)}) \rightharpoonup (y, z)$

in $W^{1,p}(\Omega;\mathbb{R}^3)\times BV(\Omega;\mathbb{R}^{M+1})$, then $(y,z)\in\mathbb{S}(t)$. Indeed, we have $z_{(j)}\to z$ in $L^1(\Omega;\mathbb{R}^{M+1})$ in our setting and hence for all $(\tilde{y},\tilde{z})\in\mathcal{Q}$, we get

$$\begin{aligned}\mathcal{E}(t,y,z) &\le \liminf_{j\to\infty}\mathcal{E}\left(t_j,y_{(j)},z_{(j)}\right)\le\liminf_{j\to\infty}\left(\mathcal{E}(t_j,\tilde{y},\tilde{z})+\mathcal{D}(z_{(j)},\tilde{z})\right)\\ &=\mathcal{E}(t,\tilde{y},\tilde{z})+\mathcal{D}(z,\tilde{z}).\end{aligned}$$

In particular, as $\mathcal{E}(t_j,\tilde{y},\tilde{z})$ is finite for some $(\tilde{y},\tilde{z})\in\mathcal{Q}$, we get $\mathcal{E}(t,y,z)<+\infty$ and thus $\det\nabla y>0$ a.e. in Ω in view of (10).

To prove injectivity, we profit again from the fact that quasistatic evolution of energetic solutions is very close to a purely static problem. In view of (21), we obtain, for each $t\in[0,T]$, all necessary convergences that were used in the proof of Corollary 3.1 to pass to the limit in conditions (18) and (19). □

5 Conclusions

We showed the existence of a solution to an evolutionary model of shape-memory alloys with gradient polyconvex stored energy density. It is a natural extension of polyconvexity, which exploits weak continuity of nonlinear minors of deformation gradients not only in Lebesgue but also in Sobolev spaces. This brings additional smoothness of volume and area element changes between the reference and deformed configuration; however, better mechanical understanding of this notion is still needed.

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