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A model for temperature-induced phase transformations in finite-strain elasticity

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Abstract

We propose a model for phase transformations that are driven by changes in the temperature. We consider the temperature as a prescribed quantity like an applied load. The model is based on the energetic formulation for rate-independent systems and thus allows for finite-strain elasticity. Time-dependent Dirichlet boundary conditions can be treated by decomposing the deformation as a composition of a given deformation satisfying the time-dependent boundary conditions and a part coinciding with the identity on the Dirichlet boundary.

1 Introduction

The mathematical modeling of shape-memory materials has attracted a lot of attention within the last twenty-five years by quite different series of work. One area was based on more phenomenological models in one or more spatial dimensions but included a thermodynamically consistent coupling to the energy equation, see [Fal80, CFV90, HM93, SZ93, ACJ96, FM96, BS96, KMS99, RS99, AP04]. The other area is treating a question of possible microstructures of equilibria by a careful analysis of the underlying microscopic crystallographic information about the different phases, see [BJ87, Bha93, Mül99, Bha03].

Only recently the latter theory was generalized to describe also the evolution of such microstructure, yet it remained restricted to the rate-independent and isothermal case, see [MT99, MTL02, MR03, Mie04a, KMR05]. However, there is also some work on rate-dependent systems respecting the correct microscopical data, see [AGR03, KO04] and the survey [Rou04].

However, a systematic mathematical study of temperature-driven phase transformation does not exist yet. Here, we want to provide some first results in this direction as there are many engineering applications using the temperature as the main control mechanism for the shape-memory effect, see e.g. [HM93, KMS99, AP04, SZ06] and [BS96, Ch. 5].

In order to be able to treat the case of finite-strain elasticity, which is modeled by polyconvex stored-energy density, we stay in the rate-independent setting, which allows us to use minimization techniques (direct method in the calculus of variations). However, this approach implies that we have to restrict the temperature fields to stationary states at each time instant $t \in [0, T]$, where t is a slow process time that moves much slower than all relaxation processes in the body. In particular, we make the modeling assumption that the temperature θ is given a priori as an “applied load” and we write $\theta = \theta_{\text{appl}}(t, x)$. Such an assumption is often used in engineering, as it is acceptable if the body is small in at least one direction like wires or plates. Then, excessive or missing heat can be

balanced through the environment. Nevertheless, $\theta_{\text{appl}}(t, \cdot)$ may be a non-constant equilibrium of the heat equation, if the temperature is fixed by heating or cooling at parts of the boundary.

Our model consists of a material that can be described by a stored-energy density $W(x, \nabla\varphi, z, \theta)$, where $x \in \Omega$ denotes the material point, $F = \nabla\varphi$ is the gradient of the deformation $\varphi : \Omega \rightarrow \mathbb{R}^d$, and $z : \Omega \rightarrow Z_M = \{(z_1, \dots, z_M) \in [0, 1]^M \mid \sum_1^M z_j = M\}$ is the phase indicator where $z_j \in [0, 1]$ gives the volume fraction of the j th phase. The energy potential then takes the form

$$\mathcal{E}(t, \varphi, z) = \int_{\Omega} W(x, \nabla\varphi, z, \theta_{\text{appl}}(t, x)) dx + \mathcal{G}(z) - \langle \ell(t), \varphi \rangle,$$

where $\ell \in C^1([0, T], W^{1,p}(\Omega)^*)$ denotes an applied loading, see (2.3), and \mathcal{G} is a regularizing term such that $\mathcal{G}(z) \sim \|z\|_{W^{\alpha,p}(\Omega)}^p$ for some $\alpha \in (0, 1/p)$.

In addition, we specify a dissipation distance \mathcal{D} on $\mathcal{Z} = L^1(\Omega; Z_M)$ in the form

$$\mathcal{D}(z_{\text{old}}, z_{\text{new}}) = \int_{\Omega} \delta(x, z_{\text{old}}(x), z_{\text{new}}(x)) dx,$$

where $\delta(x, \cdot, \cdot)$ is a (possibly unsymmetric) metric on Z_M , see (2.4). Specifying the set \mathcal{F} as those function $\varphi \in W^{1,p}(\Omega; \mathbb{R}^d)$ satisfying Dirichlet boundary data φ_{Dir} at $\Gamma_{\text{Dir}} \subset \partial\Omega$, we are able to pose our problem as the energetic formulation for rate-independent systems as in [MTL02, MaM05, Mie05]. For a given initial value $(\varphi^0, z^0) \in \mathcal{F} \times \mathcal{Z}$ we have to find a pair $(\varphi, z) : [0, T] \rightarrow \mathcal{F} \times \mathcal{Z}$ with $(\varphi(0), z(0)) = (\varphi^0, z^0)$ such that for all $t \in [0, T]$ the *global stability* (S) and the *energy balance* (E) hold

$$\begin{aligned} \text{(S)} \quad & \mathcal{E}(t, \varphi(t), z(t)) \leq \mathcal{E}(t, \widehat{\varphi}, \widehat{z}) + \mathcal{D}(z(t), \widehat{z}) \text{ for all } (\widehat{\varphi}, \widehat{z}) \in \mathcal{F} \times \mathcal{Z}, \\ \text{(E)} \quad & \mathcal{E}(t, \varphi(t), z(t)) + \text{Diss}_{\mathcal{D}}(z, [0, t]) = \mathcal{E}(0, \varphi^0, z^0) + \int_0^t \partial_s \mathcal{E}(s, \varphi(s), z(s)) ds, \end{aligned}$$

where $\text{Diss}_{\mathcal{D}}(z, [s, t])$ is defined as the supremum of $\sum_{j=1}^n \mathcal{D}(z(t_{j-1}), z(t_j))$ over all finite partitions $s \leq t_0 < t_1 < \dots < t_n \leq t$. For short, we call any such $(\varphi, z) : [0, T] \rightarrow \mathcal{F} \times \mathcal{Z}$ an *energetic solution associated with \mathcal{E} and \mathcal{D}* .

This energetic formulation is a weak form for the more familiar differential inclusions for rate-independent systems (cf. [MT04, Mie05]). Its advantage arises from the fact that it is derivative free and thus allows for a wide range of applications. In Section 2 we provide more details on the model and in Section 3 we specify the exact assumptions on the constitutive functions W and δ . The main point is that the partial derivative $\partial_t \mathcal{E}(t, \varphi, z)$ has to be defined whenever $\mathcal{E}(t, \varphi, z) < \infty$. In finite-strain elasticity we have to allow for $\mathcal{E}(t, \varphi, z) = +\infty$, namely if $\det \nabla\varphi(x) \leq 0$ on a set of positive measure. Thus, we have $\mathcal{E}(t, \varphi, z) = +\infty$ on a dense set in $[0, T] \times \mathcal{F} \times \mathcal{Z}$.

In Proposition 4.1 we will derive an estimate of the form

$$|\partial_t \mathcal{E}(t, \varphi, z)| \leq c_1^E (\mathcal{E}(t, \varphi, z) + c_0^E) \tag{1.1}$$

under the assumption that W satisfies $|\partial_{\theta} W(x, F, z, \theta)| \leq c_1^W (W(x, F, z, \theta) + c_0^W)$ and that $\partial_t \theta_{\text{appl}} \in L^{\infty}([0, T] \times \Omega)$. Using the standard coercivity and polyconvexity assumptions we

then show in Theorem 4.2 that for all stable initial data (φ^0, z^0) energetic solution exist. Here, we draw from the abstract theory developed in [MaM05, Mie05, FM06].

Finally, Section 5 treats the case of time-dependent Dirichlet boundary conditions. For this we assume that each $\varphi_{\text{Dir}}(t, \cdot)$ can be extended to a diffeomorphism from \mathbb{R}^d to \mathbb{R}^d such that $\varphi_{\text{Dir}} \in C^2([0, T] \times \mathbb{R}^d; \mathbb{R})$ and $\nabla \varphi_{\text{Dir}}, (\nabla \varphi_{\text{Dir}})^{-1} \in \text{BC}^1([0, T] \times \mathbb{R}^d; \mathbb{R}^{d \times d})$. Then, we seek $\varphi(t, \cdot)$ in the form $\varphi(t, x) = \varphi_{\text{Dir}}(t, \psi(t, x))$ with $\psi(t, \cdot) \in \tilde{\mathcal{F}}$, where

$$\tilde{\mathcal{F}} = \{ \psi \in W^{1,p}(\Omega; \mathbb{R}^d) \mid \psi|_{\Gamma_{\text{Dir}}} = \text{id} \} \quad \text{and} \quad \tilde{\mathcal{E}}(t, \psi, z) = \mathcal{E}(t, \varphi_{\text{Dir}}(t) \circ \psi, z).$$

The crucial observation in [FM06] was that $\partial_t \tilde{\mathcal{E}}(t, \psi, z)$ again satisfies an estimate of the form (1.1), if W satisfies an estimate of the form

$$|\partial_F W(x, F, z, \theta) F^T| \leq c_1^K (W(x, F, z, \theta) + c_0^K). \quad (1.2)$$

The tensor on the left-hand side is called the Kirchhoff stress tensor. Considering F as an element of the Lie group $\text{GL}_+(\mathbb{R}^d)$ we have to interpret $\partial_F W$ as an element of $\text{T}_F^* \text{GL}_+(\mathbb{R}^d)$ and $\partial_F W F^T$ lies in $\text{T}_F^* \text{GL}_+(\mathbb{R}^d) = \text{gl}(\mathbb{R}^d)^*$. We address some of these Lie group issues, which were initiated in [Mie02, Mie03], in the context of finite-strain elastoplasticity.

Using (1.2) and a similar estimate for the second derivative we are then able to transfer the isothermal existence result of [FM06] into our temperature-driven model, see Theorem 5.2.

2 The mechanical model

We consider a body with reference configuration $\Omega \subset \mathbb{R}^d$. The body may undergo deformations $\varphi : \Omega \rightarrow \mathbb{R}^d$ and phase transformations. The latter will be characterized by the internal variable $z : \Omega \rightarrow Z_M$, where Z_M is the Gibbs simplex

$$Z_M = \left\{ Z = (z_1, \dots, z_M) \in \mathbb{R}^M \mid z_j \geq 0, \sum_{m=1}^M z_m = 1 \right\} \quad (2.1)$$

The material behavior also depends on the temperature θ , which will be considered as a time dependent and possibly space dependent given parameter. Thus, we will not solve an associated heat equation, we rather treat θ as an ‘‘applied load’’ and hence write $\theta_{\text{appl}} : [0, T] \times \Omega \rightarrow \mathbb{R}$ for the given temperature profile.

This approximation for the temperature is often used in engineering models and has its justification in situations where the changes of the loading are slow and the body is small in at least one direction such that excess heat can be transported very fast to the surface and radiated into the environment. Moreover, heating at parts of the body (e.g. one end of a long wire) may give rise to a temperature profile that depends on the material points. In fact, the same arguments are used for the justification of isothermal models; hence the present work is a second step into the direction of models taking into account a full thermo-mechanical coupling.

The stored-energy density $W : \Omega \times \mathbb{R}^{d \times d} \times Z_M \times (0, \infty) \rightarrow \mathbb{R}_\infty := \mathbb{R} \cup \{\infty\}$ describes the material behavior and we obtain the *stored-energy functional*

$$\mathcal{E}(t, \varphi, z) = \int_{\Omega} W(x, \nabla \varphi(x), z(x), Q_{\text{appl}}(t, x)) dx + \mathcal{G}(z) - \langle \ell(t), \varphi \rangle, \quad (2.2)$$

where $\ell(t)$ denotes the applied mechanical loading in the form

$$\langle \ell(t), \varphi \rangle = \int_{\Omega} f_{\text{appl}}(t, x) \cdot \varphi(x) dx + \int_{\partial\Omega} g_{\text{appl}}(t, x) \cdot \varphi(x) da. \quad (2.3)$$

The term $\mathcal{G}(z)$ denotes some regularizing contribution which introduces a length scale and thus suppresses very small oscillations of the volume fractions z . As for microstructures in shape-memory alloys we expect jumps in z (e.g. at habit planes where twins of martensites meet the austenite) we choose either

$$\mathcal{G}(z) = \int_{\Omega} \kappa \|Dz\| = \sup \left\{ \kappa \int_{\Omega} z \cdot \operatorname{div} \psi dx \mid \psi \in C_c^1(\Omega; \mathbb{R}^{M \times d}), \|\psi(x)\|_* \leq 1 \text{ on } \Omega \right\}$$

(where $\|\cdot\|_*$ denotes an arbitrary norm on $\mathbb{R}^{M \times d}$) or

$$\mathcal{G}(z) = \kappa \int_{\Omega \times \Omega} \frac{|z(x) - z(y)|^p}{|x - y|^{d+p\alpha}} dx dy$$

for some $p \in (1, \infty)$ and $\alpha \in (0, 1/p)$. These terms are such that functions $z \in \mathcal{Z} = L^1(\Omega; Z_M)$ with $\mathcal{G}(z) < \infty$ lie in $BV(\Omega; \mathbb{R}^M)$ or $W^{\alpha, p}(\Omega; \mathbb{R}^M)$, respectively. These spaces embed compactly into $L^1(\Omega; \mathbb{R}^M)$ but still allow for solutions with jumps along sufficiently regular hypersurfaces in Ω . For simplicity we restrict to the case $W^{\alpha, p}(\Omega; \mathbb{R}^M)$ and refer to [Mai06] for the case using $BV(\Omega; \mathbb{R}^M)$.

For describing the hysteretic behavior of the phase transformations we use a *dissipation distance* \mathcal{D} defined on \mathcal{Z} . For this we introduce a constitutive function $\delta : \Omega \times Z_M \times Z_M \rightarrow [0, \infty)$, which satisfies for all $x \in \Omega, z_1, z_2, z_3 \in Z_M$ the estimates

$$\begin{aligned} \frac{1}{C} |z_1 - z_2| &\leq \delta(x, z_1, z_2) \leq C |z_1 - z_2|, \\ \delta(x, z_1, z_3) &\leq \delta(x, z_1, z_2) + \delta(x, z_2, z_3). \end{aligned} \quad (2.4)$$

With this we define the dissipation distance $\mathcal{D} : \mathcal{Z} \times \mathcal{Z} \rightarrow [0, \infty)$ via

$$\mathcal{D}(z_{\text{old}}, z_{\text{new}}) = \int_{\Omega} \delta(x, z_{\text{old}}(x), z_{\text{new}}(x)) dx,$$

which then satisfies $\frac{1}{C} \|z_{\text{old}} - z_{\text{new}}\|_{L^1(\Omega)} \leq \mathcal{D}(z_{\text{old}}, z_{\text{new}}) \leq C \|z_{\text{old}} - z_{\text{new}}\|_{L^1(\Omega)}$ and the triangle inequality. Note that we allow for unsymmetry, i.e. $\mathcal{D}(z_{\text{old}}, z_{\text{new}}) \neq \mathcal{D}(z_{\text{new}}, z_{\text{old}})$ may occur.

We specify the set of admissible deformations \mathcal{F} by choosing a suitable Sobolev space $W^{1, p}(\Omega; \mathbb{R}^d)$ and by describing Dirichlet data at the part Γ_{Dir} of $\partial\Omega$:

$$\mathcal{F} = \{ \varphi \in W^{1, p}(\Omega; \mathbb{R}^d) \mid (\varphi - \varphi_{\text{Dir}})|_{\Gamma_{\text{Dir}}} = 0 \},$$

where $\varphi_{\text{Dir}} \in W^{1,p}(\Omega; \mathbb{R}^d)$ is given. Throughout we assume that $p \in (1, \infty)$, Ω and Γ_{Dir} are such that there exists $C_{\Omega, \text{Dir}} > 0$ so that

$$\forall \varphi \in W^{1,p}(\Omega; \mathbb{R}^d) \text{ with } \varphi|_{\Gamma_{\text{Dir}}} = 0 : \quad \|\nabla \varphi\|_{L^p} \geq C_{\Omega, \text{Dir}} \|\varphi\|_{W^{1,p}}. \quad (2.5)$$

Finally the process is assumed to be governed by the energetic formulation of rate-independent processes as introduced in [MT99, MTL02], see also the survey in [Mie05]. A function $(\varphi, z) : [0, T] \rightarrow \mathcal{F} \times \mathcal{Z}$ is called an *energetic solution* of the rate-independent system associated with \mathcal{E} and \mathcal{D} if $\partial_t \mathcal{E}(\cdot, \varphi(\cdot), z(\cdot)) \in L^1([0, T])$ and if for all $t \in [0, T]$ we have the *global stability* (S) and the *energy balance* (E):

$$\begin{aligned} \text{(S)} \quad & \forall (\tilde{\varphi}, \tilde{z}) \in \mathcal{F} \times \mathcal{Z} : \quad \mathcal{E}(t, \varphi(t), z(t)) \leq \mathcal{E}(t, \tilde{\varphi}, \tilde{z}) + \mathcal{D}(z(t), \tilde{z}), \\ \text{(E)} \quad & \mathcal{E}(t, \varphi(t), z(t)) + \text{Diss}_{\mathcal{D}}(z, [0, t]) = \mathcal{E}(0, \varphi(0), z(0)) + \int_0^t \partial_s \mathcal{E}(s, \varphi(s), z(s)) \, ds, \end{aligned}$$

where the dissipation $\text{Diss}_{\mathcal{D}}$ is defined via

$$\text{Diss}_{\mathcal{D}}(z, [r, s]) = \sup \left\{ \sum_{j=1}^N \mathcal{D}(z(t_{j-1}), z(t_j)) \mid N \in \mathbb{N}, r \leq t_0 < t_1 < \dots < t_N \leq s \right\}.$$

We note that this energetic formulation reduces to the classical theory of *generalized standard materials* (see [Mie06]), if we assume that the solutions are sufficiently smooth and δ has the form $\delta(x, z_1, z_2) = \Delta(x, z_2 - z_1)$. Then, (S) and (E) are equivalent to

$$\begin{cases} -\text{div } \partial_F W(x, \nabla \varphi, z, \theta_{\text{appl}}) = f_{\text{appl}} & \text{in } \Omega, \\ (\varphi - \varphi_{\text{Dir}})|_{\Gamma_{\text{Dir}}} = 0, \quad \partial_F W(x, \nabla \varphi, z, \theta_{\text{appl}})n = g_{\text{appl}} & \text{on } \partial\Omega \setminus \Gamma_{\text{Dir}} \end{cases}$$

$$0 \in \partial_{\dot{z}} \Delta(x, \dot{z}) + \partial_z W(x, \nabla \varphi, z, \theta_{\text{appl}}) + D\mathcal{G}(z) \text{ in } \Omega,$$

where $\dot{z} = \frac{\partial}{\partial t} z$.

3 The mathematical assumptions

We make the assumptions more precise now. For the stored-energy density W we let $\mathbb{D} = \Omega \times \mathbb{R}^{d \times d} \times Z_M \times [\theta_{\min}, \theta_{\max}]$ and assume

$$W : \mathbb{D} \rightarrow \mathbb{R}_{\infty} \text{ is a normal integrand,} \quad (3.1)$$

i.e. for a.a. $x \in \Omega$ the function $W(x, \cdot, \cdot, \cdot)$ is lower semicontinuous and for all (F, z, θ) the function $W(\cdot, F, z, \theta)$ is measurable. We assume coercivity as follows:

$$\exists p > d \quad \exists C > 0 \quad \forall (x, F, z, \theta) \in \mathbb{D} : \quad W(x, F, z, \theta) \geq \frac{1}{C} |F|^p - C. \quad (3.2)$$

Our conditions will be compatible with the condition $W(x, F, z, \theta) = +\infty$ for $\det F \leq 0$ and $W(x, F_k, z, \theta) \rightarrow +\infty$ if $0 < \det F_k \rightarrow 0$. Moreover, they are compatible with frame

indifference, namely $W(x, RF, z, \theta) = W(x, F, z, \theta)$ for all $R \in \text{SO}(\mathbb{R}^d)$. Of course, we do not need to impose these conditions as they are not needed to prove the existence result below. However, they are physically desirable and make the mathematics much more difficult. The notion of polyconvexity was developed to handle exactly this case, see e.g. [Mül99, Bal02].

The stored-energy density W is called polyconvex in $F \in \mathbb{R}^{d \times d}$, if $W(x, \cdot, z, \theta)$ can be written as a convex function of $\mathbb{M}(F) \in \mathbb{R}^{\tau(d)}$, the vector of all minors (subdeterminants) of $F \in \mathbb{R}^{d \times d}$. For $d = 2$ we have $\mathbb{M}(F) = (F, \det F)$ with $\tau(2) = 5$ and for $d = 3$ we have $\mathbb{M}(F) = (F, \text{cof } F, \det F)$ with $\tau(3) = 19$. More precisely, we assume

$$\begin{aligned} & \exists \text{ a normal integrand } G: \Omega \times \mathbb{R}^{\tau(d)} \times Z_M \times [\theta_{\min}, \theta_{\max}] \rightarrow \mathbb{R}_{\infty} : \\ & \text{(i) } \forall (x, z, \theta) : \quad G(x, \cdot, z, \theta): \mathbb{R}^{\tau(d)} \rightarrow \mathbb{R}_{\infty} \text{ is convex,} \\ & \text{(ii) } \forall (x, F, z, \theta) \in \mathbb{D} : \quad W(x, F, z, \theta) = G(x, \mathbb{M}(F), z, \theta). \end{aligned} \quad (3.3)$$

The final conditions concern the temperature dependence of W . The applied temperature will insert or extract energy according to $\partial_{\theta} W(x, \nabla \varphi, z, \theta_{\text{appl}}) \dot{\theta}_{\text{appl}}$. To control this term we assume that θ_{appl} is smooth enough and that the derivatives $\partial_{\theta}^j W$ exist for $j = 1$ and 2 everywhere where W is finite and that these derivatives are dominated by W itself:

$$\begin{aligned} & \exists c_0^W, c_1^W > 0 \forall (x, F, z, \theta) \in \mathbb{D} \forall j \in \{1, 2\} : \\ & |\partial_{\theta}^j W(x, F, z, \theta)| \leq c_1^W (W(x, F, z, \theta) + c_0^W). \end{aligned} \quad (3.4)$$

Lemma 3.1 *If assumption (3.4) holds, then for all $(x, F, z, \theta) \in \mathbb{D}$ and all $\theta_1 \in [\theta_{\min}, \theta_{\max}]$ we have*

$$W(x, F, z, \theta_1) + c_0^W \leq e^{c_1^W |\theta_1 - \theta|} (W(x, F, z, \theta) + c_0^W).$$

Proof: We consider (x, F, z) to be fixed and define $w(\theta) = W(x, F, z, \theta) + c_0^W$. Assumption (3.4) simply means $|w'(\theta)| \leq c_1^W w(\theta)$. Thus, Gronwall's lemma yields the desired result $w(\theta_1) \leq e^{c_1^W |\theta_1 - \theta|} w(\theta)$ for all $\theta, \theta_1 \in [\theta_{\min}, \theta_{\max}]$. In particular, it is sufficient to have $w(\theta) < \infty$ at one point to conclude that w is finite on the whole interval. ■

Before using this condition for the estimate of the time derivative of the stored-energy function we discuss possible constitutive relations that satisfy all our assumptions. For simplicity we neglect any dependence on the material point $x \in \Omega$. In shape-memory models it is usual to start from the stored-energy densities of the pure phases, i.e. with $z = e_j \in \mathbb{R}^M$ for the j th phase or variant of a phase. We assume that each of these phases is described by a polyconvex stored-energy density

$$W_j : \begin{cases} \mathbb{R}^{d \times d} \times [\theta_{\min}, \theta_{\max}] & \rightarrow \mathbb{R}_{\infty} \\ (F, \theta) & \mapsto g_j(\mathbb{M}(F), \theta), \end{cases}$$

where $g_j(\cdot, \theta)$ is assumed to be continuous and convex while $g(\mathbb{M}(F), \cdot) \in C^2([\theta_{\min}, \theta_{\max}])$ or $g(\mathbb{M}(F), \cdot) \equiv +\infty$. Typical examples are of the type $W_j(F, \theta) = +\infty$ for $\det F \leq 0$ and

$$W_j(F, \theta) = a_j(\theta) |F|^p + \frac{b_j(\theta)}{(\det F)^r} + \widetilde{W}_j(F, \theta) \quad \text{for } \det F > 0, \quad (3.5)$$

where $a_j, b_j \in C^2([\theta_{\min}, \theta_{\max}]; (0, \infty))$ and the exponents satisfy $r > 0$ and $p > d$. The function $\widetilde{W}_j : \mathbb{R}^{d \times d} \times [\theta_{\min}, \theta_{\max}] \rightarrow \mathbb{R}$ is assumed to be polyconvex in F , twice differentiable in θ , and of lower order, i.e.

$$\forall i \in \{0, 1, 2\} \forall F \in \mathbb{R}^{d \times d} \forall \theta \in [\theta_{\min}, \theta_{\max}] : |\partial_\theta^i \widetilde{W}_j(F, \theta)| \leq C(1 + |F|)^{\widetilde{p}}$$

for some $C > 0$ and $\widetilde{p} < p$. In particular, the functions \widetilde{W}_j are supposed to contain the information about the anisotropies of the different phases, see [SN03] for suitable anisotropic polyconvex functions.

The final stored-energy density is now obtained by interpolating between the extremal pure phases. We may either use a linear or an exponential interpolation and in addition we may add a mixture term for penalizing phase mixtures:

$$W(F, z, \theta) = \sum_{j=1}^M z_j W_j(F, \theta) + w_{\text{mix}}(z, \theta), \quad (3.6)$$

or

$$W(F, z, \theta) = \frac{1}{\beta} \log \left(\sum_{j=1}^M z_j e^{\beta W_j(F, \theta)} \right) + w_{\text{mix}}(z, \theta), \quad (3.7)$$

where, for instance, $w_{\text{mix}}(z, \theta) = \sum_{j=1}^M \gamma_j z_j^{r_j} (1 - z_j)^{r_j}$ for $\gamma_j = \gamma_j(\theta) \geq 0$ and $r_j = r_j(\theta) > 0$. In both cases, the function $W(\cdot, z, \theta)$ inherits polyconvexity. For (3.7) we may even allow for $\beta = \beta(\theta)$ if the leading coefficients a_j and b_j for W_j in (3.5) are independent of j . Then, W in (3.7) takes the form

$$W(F, z, \theta) = a(\theta) |F|^p + \frac{b(\theta)}{(\det F)^r} + \frac{1}{\beta(\theta)} \log \left(\sum_{j=1}^M z_j e^{\beta(\theta) \widetilde{W}_j(F, \theta)} \right) + w_{\text{mix}}(z, \theta).$$

In conclusion, this shows that based on standard polyconvex materials it is easily possible to construct stored-energy densities satisfying the above assumptions.

4 The main existence result

For a given temperature profile θ_{appl} and a given external loading ℓ with

$$\begin{aligned} \theta_{\text{appl}} &\in C^1([0, T]; L^\infty(\Omega; [\theta_{\min}, \theta_{\max}])) \text{ and} \\ \ell &\in C^1([0, T]), W^{1,p}(\Omega; \mathbb{R}^d)^* \end{aligned} \quad (4.1)$$

we now study the stored-energy functional \mathcal{E} as defined in (2.2).

Proposition 4.1 *Under the above assumptions the following holds:*

- (a) *If for some $(t_*, \varphi, z) \in [0, T] \times \mathcal{F} \times \mathcal{Z}$ we have $\mathcal{E}(t_*, \varphi, z) < \infty$, then $\mathcal{E}(\cdot, \varphi, z) \in C^1([0, T])$ and $\partial_t \mathcal{E}(t, \varphi, z) = \int_\Omega \partial_\theta W(\nabla \varphi, z, \theta_{\text{appl}}(t)) \dot{\theta}_{\text{appl}}(t) dx - \langle \dot{\ell}(t), \varphi \rangle$.*

(b) There exist constants $c_0^E, c_1^E > 0$, such that $\mathcal{E}(t, \varphi, z) < \infty$ implies $|\partial_t \mathcal{E}(t, \varphi, z)| \leq c_1^E(\mathcal{E}(t, \varphi, z) + c_0^E)$.

(c) For each $E_* \in \mathbb{R}$ and $\varepsilon > 0$ there exists $\delta > 0$ such that $\mathcal{E}(t_1, \varphi, z) \leq E_*$ and $|t_1 - t_2| < \delta$ imply $|\partial_t \mathcal{E}(t_1, \varphi, z) - \partial_t \mathcal{E}(t_2, \varphi, z)| < \varepsilon$.

Proof: We first use the coercivity (3.2) to find

$$\mathcal{E}(t_*, \varphi, z) \geq \frac{1}{C} \|\nabla \varphi\|_{L^p}^p - C|\Omega| - \|\ell(t_*)\| \|\varphi\|_{W^{1,p}}.$$

Using (2.5) we obtain $c_0, C_0 > 0$ such that

$$\mathcal{E}(t_*, \varphi, z) \geq c_0 \|\varphi\|_{W^{1,p}}^p - C_0. \quad (4.2)$$

To show differentiability with respect to t we use $\theta_{\text{appl}} \in C^1([0, T]; L^\infty(\Omega; [\theta_{\min}, \theta_{\max}]))$ and condition (3.4). For $h \neq 0$ and $t_* + h \in [0, T]$ the mean-value theorem provides some $s \in [0, 1]$ such that

$$\begin{aligned} \frac{1}{h}(\mathcal{E}(t_*+h, \varphi, z) - \mathcal{E}(t_*, \varphi, z)) &= \\ \int_{\Omega} \partial_{\theta} W(x, \nabla \varphi, z, \theta_{\text{appl}}(t_*+sh, x)) \partial_t \theta_{\text{appl}}(t_*+sh, x) dx &- \langle \frac{1}{h}(\ell(t+h) - \ell(t)), \varphi \rangle. \end{aligned}$$

Using $\mathcal{E}(t_*, \varphi, z) < \infty$ and Lemma 3.1 we know that $|\partial_{\theta} W(x, \nabla \varphi(x), z(x), \tilde{\theta}(x))| \leq g(x)$, a.e. on Ω for some $\tilde{g} \in L^1(\Omega)$, where $\tilde{\theta} \in L^\infty(\Omega; [\theta_{\min}, \theta_{\max}])$ is arbitrary. Since $\partial_t \theta \in C^0([0, T]; L^\infty(\Omega))$ we may pass to the limit $h \rightarrow \infty$ by the Lebesgue theorem and part (a) is proved.

For part (b) we use the representation of part (a) and estimate as follows

$$|\partial_t \mathcal{E}(t, \varphi, z)| \leq \int_{\Omega} |\partial_{\theta} W(x, \nabla \varphi, z)| dx \|\partial_t \theta_{\text{appl}}\|_{\infty} + \|\dot{\ell}(t)\|_* \|\varphi\|_{W^{1,p}}.$$

Using (3.4) for $j = 1$ and (4.2) the desired result follows immediately.

For part (c) we use (3.4) for $j = 2$ and (4.1), which implies

$$\|\dot{\ell}(t_1) - \dot{\ell}(t_2)\|_* + \|\partial_t \theta(t_1 \cdot) - \partial_t \theta(t_2, \cdot)\|_{L^\infty(\Omega)} \leq \omega(|t_1 - t_2|), \quad (4.3)$$

where $\omega: [0, \infty) \rightarrow [0, \infty)$ is a continuous modulus of continuity with $\omega(0) = 0$. We obtain

$$\begin{aligned} &|\partial_t \mathcal{E}(t_1, \varphi, z) - \partial_t \mathcal{E}(t_2, \varphi, z)| \\ &\leq \int_{\Omega} |\partial_{\theta} W(x, \nabla \varphi, z, \theta(t_1)) - \partial_{\theta} W(x, \nabla \varphi, z, \theta(t_2))| \|\partial_t \theta(t_1)\|_{\infty} dx \\ &\quad + \int_{\Omega} |\partial_{\theta} W(x, \nabla \varphi, z, \theta(t_2))| \|\partial_t \theta(t_1) - \partial_t \theta(t_2)\|_{\infty} dx + \|\dot{\ell}(t_1) - \dot{\ell}(t_2)\|_* \|\varphi\|_{W^{1,p}} \\ &\leq \int_{\Omega} c_1^W [W(x, \nabla \varphi, z, \theta(t_1+s(t_2-t_1))) + c_0] \|\theta(t_1) - \theta(t_2)\|_{\infty} dx \|\partial_t \theta\|_{\infty} \\ &\quad + \tilde{C}(\mathcal{E}(t, \varphi, z) + c_0^E) \omega(t_1 - t_2) \\ &\leq \hat{C}(E_* + c_0^E)(|t_1 - t_2| + \omega(t_1 - t_2)). \end{aligned}$$

Thus, the proposition is established. ■

We now show that the energetic formulation (S) & (E) introduced in Section 2 has at least one solution $q = (\varphi, z) : [0, T] \rightarrow \mathcal{Q} = \mathcal{F} \times \mathcal{Z}$, for a given stable initial datum $q^0 \in \mathcal{Q}$. Here q^0 is called *stable* if it satisfies the (static) condition (S) at time $t = 0$. The existence theory relies on the abstract framework developed in [MaM05] with the recent refinements derived in [Mie05, FM06]. These refinements are based on the selection technique and an approximation result of Lebesgue integrals via Riemann sums developed in [DFT05].

Here we do not go into the details of the proof of the abstract result. We just mention that the theory is based on time-incremental minimization problems for sequences of partitions $0 = t_0^k < t_1^k < \dots < t_{N_k-1}^k < t_{N_k}^k = T$ in the form:

$$(IP)_k \quad \begin{cases} \text{Given } q^0 \in \mathcal{Q}, \text{ find iteratively } q_1^k, \dots, q_{N_k}^k \in \mathcal{Q} \text{ such that} \\ q_j^k \text{ minimizes } \tilde{q} \mapsto \mathcal{E}(t_j^k, \tilde{q}) + \mathcal{D}(q_{j-1}^k, \tilde{q}). \end{cases}$$

Thus, for each k we may define the piecewise constant interpolant $\bar{q}^k : [0, T] \rightarrow \mathcal{Q}$ with $\bar{q}^k(t) = q_j^k$ for $t \in [t_j^k, t_{j+1}^k)$ for $j = 0, \dots, N_k$.

Theorem 4.2 *Let $\mathcal{Q} = \mathcal{F} \times \mathcal{Z}$ be as specified above and let \mathcal{E} and \mathcal{D} satisfy the assumptions from above. Then, for each stable $q^0 \in \mathcal{Q}$ there exists an energetic solution $q^0 : [0, T] \rightarrow \mathcal{Q}$ with $q(0) = q^0$. This solution $q = (\varphi, z)$ satisfies*

$$\begin{aligned} \varphi &\in L^\infty([0, T], W^{1,p}(\Omega; \mathbb{R}^d)) \text{ and} \\ z &\in L^\infty([0, T], W^{\alpha,2}(\Omega; \mathbb{R}^M) \cap BV([0, T]; L^1(\Omega, \mathbb{R}^m))), \end{aligned}$$

and it can be obtained as the limit of a subsequence $(\bar{q}^{k_l})_{l \in \mathbb{N}}$ of the above interpolants associated with $(IP)_k$ as follows:

- (i) $\forall t \in [0, T] : \bar{z}^{k_l}(t) \rightharpoonup z(t) \text{ in } W^{\alpha,2}(\Omega; \mathbb{R}^M),$
- (ii) $\forall t \in [0, T] : \mathcal{E}(t, \bar{q}^{k_l}(t)) \rightarrow \mathcal{E}(t, q(t))$
- (iii) $\forall t \in [0, T] : \text{Diss}_{\mathcal{D}}(\bar{q}^{k_l}, [0, t]) \rightarrow \text{Diss}_{\mathcal{D}}(q, [0, t])$
- (iv) $\forall t \in [0, T] \exists \text{ subseq. } (k_n^t)_{n \in \mathbb{N}} \text{ of } (k_l)_{l \in \mathbb{N}} : \bar{\varphi}^{k_n^t}(t) \rightharpoonup \varphi(t) \text{ in } W^{1,p}(\Omega; \mathbb{R}^d).$

The main point in passing to the limit is the use of the weak lower semicontinuity of $\mathcal{E}(t, \cdot)$ on \mathcal{Q} considered as a convex subset of $W^{1,p}(\Omega; \mathbb{R}^d) \times W^{\alpha,2}(\Omega; \mathbb{R}^M)$. The dissipation behaves better as it is strongly continuous in $L^1(\Omega)$ and hence weakly continuous in $\mathcal{Z} = W^{\alpha,2}(\Omega; Z_M)$. Together with the good dependence on the time t , which was derived in Proposition 4.1, we have fulfilled all assumptions of the abstract theory in [FM06, Sect.3]. This proves our Theorem 4.2.

5 Time-dependent Dirichlet conditions, compositions, and Lie groups

So far we have studied the situation that the boundary conditions φ_{Dir} on $\Gamma_{\text{Dir}} \subset \partial\Omega$ are independent of time. Hence, the space \mathcal{F} of admissible deformations could be chosen independent of time as well. Of course, typical practical situations lead to cases where φ_{Dir} depends on time.

The usual treatments of time-dependent boundary data involve either the additive split $\varphi(t) = \varphi_{\text{Dir}}(t) + u$, where u can then be chosen in a fixed space, or a replacement of the “hard constraint” $\varphi - \varphi_{\text{Dir}}(t)|_{\Gamma_{\text{Dir}}} \equiv 0$ by the penalization $\frac{1}{\delta} \int_{\Gamma_{\text{Dir}}} |\varphi - \varphi_{\text{Dir}}(t)|^2 da$, which is added to the energy functional. The latter method would be applicable in our case of finite-strain elasticity. However, it has the disadvantage that the treatment of the limit $\delta \rightarrow 0$ is not so easy and it is rather awkward to control the work done by the changing boundary condition. The additive split $\varphi = \varphi_{\text{Dir}} + u$ does not work here, as in finite-strain elasticity the additive split of the deformation gradient $F = \nabla\varphi = \nabla\varphi_{\text{Dir}} + \nabla u$ is not compatible with the blow-up of the stored-energy density W near $\det F = 0$.

Instead we follow the approach in [FM06, Sect.5] and use the composition

$$\varphi(t, x) = \varphi_{\text{Dir}}(t, \psi(t, x)) = (\varphi_{\text{Dir}}(t, \cdot) \circ \psi(t))(x) \quad (5.1)$$

that leads to a multiplicative split of the deformation gradient

$$F = \nabla\varphi(t, x) = \nabla\varphi_{\text{Dir}}(t, \psi(t, x))\nabla\psi(t, x). \quad (5.2)$$

To make the following analysis rigorous we assume that $\varphi_{\text{Dir}}(t, \cdot)$ can be smoothly extended onto all of \mathbb{R}^d such that it is in fact a diffeomorphism. More precisely, we assume

$$\begin{aligned} \varphi_{\text{Dir}} &\in C^1([0, T] \times \mathbb{R}^d; \mathbb{R}^d), \quad \nabla\varphi_{\text{Dir}} \in \text{BC}^1([0, T] \times \mathbb{R}^d; \mathbb{R}^{d \times d}), \\ \nabla\varphi_{\text{Dir}}(t, x) &\in \text{GL}_+(\mathbb{R}^d) \text{ for all } (t, x) \text{ and } (\nabla\varphi_{\text{Dir}})^{-1} \in \text{BC}^0([0, T] \times \mathbb{R}^d; \mathbb{R}^{d \times d}). \end{aligned} \quad (5.3)$$

Clearly, we have $\varphi(t, x) = \varphi_{\text{Dir}}(t, x)$ for $x \in \Gamma_{\text{Dir}}$ if and only if $\psi(t, x) = x$ for $x \in \Gamma_{\text{Dir}}$. Hence, we let

$$\tilde{\mathcal{F}} = \{ \psi \in W^{1,p}(\Omega; \mathbb{R}^d) \mid (\psi - \text{id})|_{\Gamma_{\text{Dir}}=0} \}$$

With the notations from the previous sections we then define $\tilde{\mathcal{Q}} = \tilde{\mathcal{F}} \times \mathcal{Z}$ and

$$\tilde{\mathcal{E}}(t, \psi, z) = \mathcal{E}(t, \varphi_{\text{Dir}}(t) \circ \psi, z)$$

and keep $\mathcal{D} : \mathcal{Z} \times \mathcal{Z} \rightarrow [0, \infty)$ as above.

The crucial condition that is needed for controlling the time derivative $\partial_t \tilde{\mathcal{E}}$ involves the Kirchhoff stress tensor

$$K(x, F, z, \theta) = \partial_F W(x, F, z, \theta) F^T \in \mathbb{R}^{d \times d}.$$

In finite-strain elasticity it is advantageous and illuminating to consider $F = \nabla\varphi$ as an element of the Lie group

$$\text{GL}_+(\mathbb{R}^d) = \{ G \in \mathbb{R}^{d \times d} \mid G^{-1} \text{ exists and } \det G > 0 \}.$$

Then, the Kirchoff tensor turns out to be the left multiplicative derivative, viz.,

$$K(x, F, z, \theta)[H] = \lim_{\varepsilon \rightarrow 0} \frac{d}{d\varepsilon} W(x, e^{\varepsilon H} F, z, \theta) = \partial_F W(x, F, z, \theta)[HF].$$

In particular, we see that $K(x, F, z, \theta)$ is an element of $\mathfrak{gl}(\mathbb{R}^d)^*$, where $\mathfrak{gl}(\mathbb{R}^d) = T_I \text{GL}_+(\mathbb{R}^d)$ is the Lie algebra of $\text{GL}_+(\mathbb{R}^d)$.

Following [FM06] (see also [Bal02]) we assume that in all points $(x, F, z, \theta) \in \mathbb{D}$ with $W(x, F, z, \theta) < \infty$ the function W is twice differentiable in F such that

$$\exists c_0^K, c_1^K > 0 \quad \forall (x, F, z, \theta) \in \mathbb{D} \quad \forall H \in \mathbb{R}^{d \times d} :$$

$$\|K(x, F, z, \theta)\|_* \leq c_1^K (W(x, F, z, \theta) + c_0^K), \quad (5.4a)$$

$$\|\partial_F K(x, F, z, \theta)[HF]\|_* \leq c_1^K (W(x, F, z, \theta) + c_0^K) \|H\|, \quad (5.4b)$$

where $\|\cdot\|$ is an arbitrary norm on $\mathfrak{gl}(\mathbb{R}^d)$ and $\|\cdot\|_*$ is the dual norm on $\mathfrak{gl}(\mathbb{R}^d)^*$.

To illuminate the (multiplicative) Lie group structure further, we omit temporarily the variables x, z , and θ . The following Lemma 5.1 states that condition (5.4a) is equivalent to global Lipschitz continuity of $\log(W + c_0^K): \text{GL}_+(\mathbb{R}^d) \rightarrow [0, \infty)$ with respect to the right-invariant distance

$$d_{\text{GL}}(F_0, F_1) = \inf \left\{ \int_0^1 \|\dot{G}(t)G(t)^{-1}\| dt \mid G \in C^1([0, 1]; \text{GL}_+(\mathbb{R}^d)), \right. \\ \left. G(0) = F_0, G(1) = F_1 \right\}. \quad (5.5)$$

This definition easily gives the right-invariance $d_{\text{GL}}(F_0 F, F_1 F) = d_{\text{GL}}(F_0, F_1)$ for all $F_0, F_1, F \in \text{GL}_+(\mathbb{R}^d)$.

Lemma 5.1 *For $W \in C^1(\text{GL}_+(\mathbb{R}^d), \mathbb{R})$ the bound in (5.4a) is equivalent to*

$$\forall F_0, F_1 \in \text{GL}_+(\mathbb{R}^d) : \quad \left| \log(W(F_0) + c_0^K) - \log(W(F_1) + c_0^K) \right| \leq c_1^K d_{\text{GL}}(F_0, F_1). \quad (5.6)$$

Proof: Equation (5.6) follows from (5.4a) by differentiating of $w(t) = \log(W(F(t)) + c_0^K)$ with respect to time, where $t \mapsto F(t)$ is the geodesic connecting F_0 and F_1 . Then,

$$\dot{w}(t) = \frac{\partial_F W(F(t))[\dot{F}(t)]}{W(F(t)) + c_0^K} = \frac{K(F(t)) : (\dot{F}(t)F(t)^{-1})}{W(F) + c_0^K} \leq c_1^K \|\dot{F}(t)F(t)^{-1}\|$$

and integration yields (5.6). For the opposite conclusion we use that

$$\frac{1}{\varepsilon} d_{\text{GL}}(F, F + \varepsilon \widehat{F}) \rightarrow \|\widehat{F}F^{-1}\| \quad \text{for } \varepsilon \rightarrow 0.$$

With $\widehat{F} = HF$ and (5.6) for $F_0 = F_1$ and $F_1 = F + \varepsilon \widehat{F}$ we find, after division by ε and taking the limit $\varepsilon \rightarrow 0$,

$$\frac{\partial_F W(F)[HF]}{W(F) + c_0^K} \leq c_1^K \|H\|.$$

As $H \in \mathbb{T}_F \text{GL}_+(\mathbb{R}^d)$ is arbitrary, this implies (5.4a). \blacksquare

The conditions (5.4) are in fact satisfied by many polyconvex stored-energy densities, for instance for Ogden materials. Consider

$$W(F) = \alpha|F|^p + \frac{\beta}{(\det F)^r} \quad \text{with } \alpha, \beta, r > 0 \text{ and } p \geq 2.$$

Then, the Kirchhoff tensor takes the form

$$K(F) = \alpha p|F|^{p-2} F F^T - \frac{\beta r}{(\det F)^r} I$$

and it is easy to establish (5.4) with $c_0^K = 0$ and $c_1^K = \max\{p, r\}$.

Unfortunately, there is nothing known about the interplay of condition (5.6) and polyconvexity. In particular, for applications in finite-strain elastoplasticity (cf. [Mie02, Mie03, Mie04b, MiM06, GM*06]) it would be interesting to know whether there exists $c_1^K > 0$ such that the function

$$F \mapsto e^{c_1^K d_{\text{GL}}(I, F)}$$

is polyconvex on $\mathbb{R}^{d \times d}$, when extended by $+\infty$ outside of $\text{GL}_+(\mathbb{R}^d)$. This question also involves the choice of the norm $\|\cdot\|$ on $\text{gl}(\mathbb{R}^d)$ used in (5.5). The only positive result is based on the seminorm

$$\|\xi\| = \|\xi + \xi^\top\|_F \quad \text{with} \quad \|\eta\|_F^2 = \eta:\eta,$$

see [MiM06].

It is easy to see that the definitions of $\tilde{\mathcal{Q}} = \tilde{\mathcal{F}} \times \mathcal{Z}$, $\tilde{\mathcal{E}} : [0, T] \times \tilde{\mathcal{Q}} \rightarrow \mathbb{R}_\infty$, and $\mathcal{D} : \mathcal{Z} \times \mathcal{Z} \rightarrow [0, \infty)$ make $\tilde{\mathcal{E}}(t, \cdot)$ and \mathcal{D} weakly lower semicontinuous with respect to the strong topology of $W^{1,p}(\Omega; \mathbb{R}^d) \times W^{\alpha,2}(\Omega; Z_M)$. Moreover, \mathcal{D} is even weakly continuous. Thus, the remaining properties to be established involve the time derivative of $\partial_t \tilde{\mathcal{E}}$, i.e. the power of the external loading which now includes the forces $f_{\text{appl}}, g_{\text{appl}}$, the temperature θ_{appl} , and the Dirichlet boundary data φ_{Dir} .

For the time derivative of $W(x, (\nabla \varphi_{\text{Dir}}) \nabla \psi, z, \theta_{\text{appl}}(t))$ we obtain the old term involving $\dot{\theta}_{\text{appl}}(t)$ and a new term involving $\nabla \dot{\varphi}_{\text{Dir}}$, namely

$$\begin{aligned} & \partial_F W(x, \nabla \varphi_{\text{Dir}} \nabla \psi, z, \theta_{\text{appl}}(t)) : [\nabla \dot{\varphi}_{\text{Dir}} \nabla \psi] \\ &= \left[\partial_F W(x, \nabla \varphi_{\text{Dir}} \nabla \psi, z, \theta_{\text{appl}}(t)) (\nabla \varphi_{\text{Dir}} \nabla \psi)^\top \right] : \left[\nabla \dot{\varphi}_{\text{Dir}} \nabla \psi (\nabla \varphi_{\text{Dir}} \nabla \psi)^{-1} \right] \\ &= K(x, \nabla \varphi_{\text{Dir}} \nabla \psi, z, \theta_{\text{appl}}(t)) : [\nabla \dot{\varphi}_{\text{Dir}} (\nabla \varphi_{\text{Dir}})^{-1}] \end{aligned}$$

where we have used the identity $A:B = (AC^\top):(BC^{-1})$. Hence, in analogy to Proposition 4.1 we obtain the following formula by the help of the assumption (5.4a):

$$\begin{aligned} \partial_t \tilde{\mathcal{E}}(t, \psi, z) &= \int_\Omega K(x, \nabla \varphi_{\text{Dir}} \nabla \psi, z, \theta_{\text{appl}}(t)) : [\nabla \dot{\varphi}_{\text{Dir}} (\nabla \varphi_{\text{Dir}})^{-1}] dx \\ &\quad + \int_\Omega \partial_\theta W(\nabla \varphi_{\text{Dir}} \nabla \psi, z, \theta_{\text{appl}}(t)) \dot{\theta}_{\text{appl}}(t) dx \\ &\quad - \langle \dot{\ell}(t), \varphi_{\text{Dir}} \rangle - \langle \ell(t), \dot{\varphi}_{\text{Dir}} \rangle, \end{aligned}$$

where $\varphi_{\text{Dir}}, \nabla\varphi_{\text{Dir}}$ and $\dot{\varphi}_{\text{Dir}} = \partial_t\varphi_{\text{Dir}}$ are evaluated at $(t, \psi(x))$. Using (5.3) we find $\nabla\dot{\varphi}_{\text{Dir}}(\nabla\varphi_{\text{Dir}})^{-1} \in C^0([0, T] \times \bar{\Omega}; \mathbb{R}^{d \times d})$ and obtain the desired estimate

$$|\partial_t \tilde{\mathcal{E}}(t, \psi, z)| \leq \tilde{c}_1^E (\tilde{\mathcal{E}}(t, \psi, z) + \tilde{c}_0^E).$$

Moreover, employing (5.4b) as in [FM06, Sect.5] and the results of Proposition 4.1 we find for each $E_* \in \mathbb{R}$ and each $\varepsilon > 0$ a $\delta > 0$ such that $\tilde{\mathcal{E}}(t_1, \psi, z) \leq E_*$ and $|t_1 - t_2| < \delta$ implies $|\partial_t \tilde{\mathcal{E}}(t_1, \psi, z) - \partial_t \tilde{\mathcal{E}}(t_2, \psi, z)| < \varepsilon$. Hence, the existence result of Section 4 can be generalized to the case of time dependent boundary conditions as follows without any change in the proof.

Theorem 5.2 *Let $\tilde{\mathcal{Q}} = \tilde{\mathcal{F}} \times \mathcal{Z}, \tilde{\mathcal{E}}$ and \mathcal{D} be as specified above. Let all the assumptions of Section 3 hold and, additionally, (5.3) and (5.4). Then, for each stable initial state $(\psi^0, z^0) \in \tilde{\mathcal{Q}}$ there exists an energetic solution $(\psi, z) : [0, T] \rightarrow \tilde{\mathcal{Q}}$ associated with the functionals $\tilde{\mathcal{E}}$ and \mathcal{D} satisfying $(\psi(0), z(0)) = (\psi^0, z^0)$.*

Moreover, this solution satisfies all the properties stated in Theorem 4.2 analogously.

6 Discussion

We have shown that the previously developed isothermal models for the hysteretic behavior for phase transformations in shape-memory alloys can be transferred to the case where the temperature is varying but given in advance. The aim was to show that the model is still capable to handle finite-strain elasticity.

There are several reasons why a true thermodynamically consistent coupling to the energy equations is still out of the reach of a rigorous mathematical treatment. One major reason is that almost all theory of finite-strain elasticity is related to the direct method of calculus of variations. Thus, we do not know whether the constructed global minimizers for polyconvex materials laws satisfy the equilibrium equations (cf. [Bal02]) and whether they are unique. See [KS84, KTW03, Kno06] for a series of uniqueness results in the static and dynamical case.

Using global minimization we have to expect that the energetic solutions as discussed above have jumps as functions of time. In a truly coupled thermo-mechanical model this would provide an instant release of energy which could not be controlled without knowing the “jump path”. If suitable uniqueness conditions, at least in certain relevant regimes, would be available then it should be possible to show that no jumps occur. In fact it is the purpose of the mesoscopical models using the phase fractions $z(t, x) \in Z_M$ to devise smoother models. In the case of small strains, see e.g., [AP04, SZ06, AMS06], there is much more hope to treat suitable models with correct coupling between temperature changes and phase transformations.

References

- [ACJ96] R. ABEYARATNE, C.-H. CHU, and R. JAMES. Kinetics of materials with wiggly energies: theory and application to the evolution of twinning microstructures in a Cu-Al-Ni shape memory alloy. *Phil. Mag. A*, 73, 457–497, 1996.
- [AGR03] M. ARNDT, M. GRIEBEL, and T. ROUBÌČEK. Modelling and numerical simulation of martensitic transformation in shape memory alloys. *Cont. Mech. Thermodyn.*, 15, 463–485, 2003.
- [AMS06] F. AURICCHIO, A. MIELKE, and U. STEFANELLI. A rate-independent model for the isothermal quasi-static evolution of shape-memory materials. *M³AS Math. Models Meth. Appl. Sci.*, 2006.
- [AP04] F. AURICCHIO and L. PETRINI. A three-dimensional model describing stress-temperature induced solid phase transformations. part ii: thermomechanical coupling and hybrid composite applications. *Int. J. Numer. Meth. Engrg.*, 61, 716–737, 2004.
- [Bal02] J. M. BALL. Some open problems in elasticity. In P. Newton, P. Holmes, and A. Weinstein, editors, *Geometry, Mechanics, and Dynamics*, pages 3–59. Springer, New York, 2002.
- [Bha93] K. BHATTACHARYA. Comparison of the geometrically nonlinear and linear theories of martensitic transformation. *Contin. Mech. Thermodyn.*, 5(3), 205–242, 1993.
- [Bha03] K. BHATTACHARYA. *Microstructure of Martensite. Why it Forms and How it Gives Rise to the Shape-Memory Effect*. Oxford University Press, New York, 2003.
- [BJ87] J. M. BALL and R. D. JAMES. Fine phase mixtures as minimizers of energy. *Arch. Rational Mech. Anal.*, 100(1), 13–52, 1987.
- [BS96] M. BROKATE and J. SPREKELS. *Hysteresis and Phase Transitions*. Springer-Verlag, New York, 1996.
- [CFV90] P. COLLI, M. FRÉMOND, and A. VISINTIN. Thermo-mechanical evolution of shape memory alloys. *Quart. Appl. Math.*, 48, 31–47, 1990.
- [DFT05] G. DAL MASO, G. FRANCFORT, and R. TOADER. Quasistatic crack growth in nonlinear elasticity. *Arch. Ratioanl Mech. Anal.*, 176, 165–225, 2005.
- [Fal80] F. FALK. Model free energy, mechanics and thermodynamics of shape memory alloys. *Acta Metall.*, 1980.
- [FM96] M. FRÉMOND and S. MIYAZAKI. *Shape Memory Alloys*. Springer-Verlag, Wien, 1996.
- [FM06] G. FRANCFORT and A. MIELKE. Existence results for a class of rate-independent material models with nonconvex elastic energies. *J. reine angew. Math.*, 595, 55–91, 2006.
- [GM*06] E. GÜRSES, A. MAINIK, C. MIEHE, and A. MIELKE. Analytical and numerical methods for finite-strain elastoplasticity. In Helmig et al. [HMW06], pages 443–481. WIAS Preprint <http://www.wias-berlin.de/publications/preprints/1127>.

- [HM93] Y. HUO and I. MÜLLER. Nonequilibrium thermodynamics of pseudoelasticity. *Contin. Mech. Thermodyn.*, 5(3), 163–204, 1993.
- [HMW06] R. Helmig, A. Mielke, and B. I. Wohlmuth, editors. *Multifield Problems in Solid and Fluid Mechanics*, volume 28 of *Lecture Notes in Applied and Computational Mechanics*. Springer-Verlag, Berlin, 2006. (Final Report of SFB 404). XI+571 pp.
- [KMR05] M. KRUŽÍK, A. MIELKE, and T. ROUBÍČEK. Modelling of microstructure and its evolution in shape-memory-alloy single-crystals, in particular in CuAlNi. *Meccanica*, 40, 389–418, 2005.
- [KMS99] M. S. KUCZMA, A. MIELKE, and E. STEIN. Modelling of hysteresis in two-phase systems. *Archive of Mechanics (Warsawa)*, 51, 693–715, 1999.
- [Kno06] R. J. KNOPS. On local uniqueness in nonlinear elastodynamics. *Quart. Appl. Math.*, 64, 321–333, 2006.
- [KO04] M. KRUŽÍK and F. OTTO. A phenomenological model for hysteresis in polycrystalline shape memory alloys. *Z. angew. Math. Mech. (ZAMM)*, 84, 835–842, 2004.
- [KS84] R. J. KNOPS and C. A. STUART. Quasiconvexity and uniqueness of equilibrium solutions in nonlinear elasticity. *Arch. Rational Mech. Anal.*, 86, 233–249, 1984.
- [KTW03] R. J. KNOPS, C. TRIMARCO, and H. T. WILLIAMS. Uniqueness and complementary energy in nonlinear elastostatics. *Meccanica*, 38, 519–534, 2003.
- [Mai06] A. MAINIK. A rate-independent model for phase transformations in shape-memory alloys. *Archive Rational Mech. Analysis*, 2006. To appear (Universität Stuttgart, SFB404 Preprint 2006/04).
- [MaM05] A. MAINIK and A. MIELKE. Existence results for energetic models for rate-independent systems. *Calc. Var. PDEs*, 22, 73–99, 2005.
- [Mie02] A. MIELKE. Finite elastoplasticity, Lie groups and geodesics on $SL(d)$. In P. Newton, A. Weinstein, and P. J. Holmes, editors, *Geometry, Dynamics, and Mechanics*, pages 61–90. Springer-Verlag, 2002.
- [Mie03] A. MIELKE. Energetic formulation of multiplicative elasto-plasticity using dissipation distances. *Cont. Mech. Thermodynamics*, 15, 351–382, 2003.
- [Mie04a] A. MIELKE. Deriving new evolution equations for microstructures via relaxation of variational incremental problems. *Comput. Methods Appl. Mech. Engrg.*, 193, 5095–5127, 2004.
- [Mie04b] A. MIELKE. Existence of minimizers in incremental elasto-plasticity with finite strains. *SIAM J. Math. Analysis*, 36, 384–404, 2004.
- [Mie05] A. MIELKE. Evolution in rate-independent systems (Ch. 6). In C. Dafermos and E. Feireisl, editors, *Handbook of Differential Equations, Evolutionary Equations, vol. 2*, pages 461–559. Elsevier B.V., Amsterdam, 2005.
- [Mie06] A. MIELKE. A mathematical framework for generalized standard materials in the rate-independent case. In Helmig et al. [HMW06], pages 351–379. WIAS Preprint <http://www.wias-berlin.de/publications/preprints/1123>.

- [MiM06] A. MIELKE and S. MÜLLER. Lower semicontinuity and existence of minimizers for a functional in elastoplasticity. *ZAMM Z. angew. Math. Mech.*, 86, 233–250, 2006.
- [MR03] A. MIELKE and T. ROUBÍČEK. A rate-independent model for inelastic behavior of shape-memory alloys. *Multiscale Model. Simul.*, 1, 571–597, 2003.
- [MT99] A. MIELKE and F. THEIL. A mathematical model for rate-independent phase transformations with hysteresis. In H.-D. Alber, R. Balean, and R. Farwig, editors, *Proceedings of the Workshop on “Models of Continuum Mechanics in Analysis and Engineering”*, pages 117–129. Shaker-Verlag, 1999.
- [MT04] A. MIELKE and F. THEIL. On rate-independent hysteresis models. *Nonl. Diff. Eqns. Appl. (NoDEA)*, 11, 151–189, 2004. (Accepted July 2001).
- [MTL02] A. MIELKE, F. THEIL, and V. I. LEVITAS. A variational formulation of rate-independent phase transformations using an extremum principle. *Arch. Rational Mech. Anal.*, 162, 137–177, 2002. (Essential Science Indicator: Emerging Research Front, August 2006).
- [Mül99] S. MÜLLER. Variational models for microstructure and phase transitions. In *Calculus of Variations and Geometric Evolution Problems (Cetraro, 1996)*, pages 85–210. Springer, Berlin, 1999.
- [Rou04] T. ROUBÍČEK. Models of microstructure evolution in shape memory alloys. In P. Ponte Castaneda, J. Telega, and B. Gambin, editors, *Nonlinear Homogenization and its Applications to Composites, Polycrystals and Smart Materials*, pages 269–304. Kluwer, 2004. NATO Sci. Series II/170.
- [RS99] K. RAJAGOPAL and A. SRINIVASA. On the thermomechanics of shape memory wires. *Z. angew. Math. Phys.*, 50(3), 459–496, 1999.
- [SN03] J. SCHRÖDER and P. NEFF. Invariant formulation of hyperelastic transverse isotropy based on polyconvex free energy functions. *Int. J. Solids Structures*, 40, 401–445, 2003.
- [SZ93] J. SPREKELS and S. M. ZHENG. Global smooth solutions to a thermodynamically consistent model of phase-field type in higher space dimensions. *J. Math. Anal. Appl.*, 176, 200–223, 1993.
- [SZ06] E. STEIN and O. ZWICKERT. Theory and finite element computations of a unified cyclic phase transformation model for monocrystalline materials at small strains. *Int. J. Comp. Mechanics*, 2006. In print.